

C₆₀ as Electron Acceptor and Donor: A Comparative DFT Study of Li@C₆₀ and F@C₆₀

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Fullerene (C₆₀) is a stable prototype system for a special class of nanomaterials. In this work, the smallest alkali metal (Li) and halogen (F) atoms were encapsulated in the C₆₀ cage, and comparative quantum chemical calculations (QCCs) were performed on their various properties using a density functional theory approach. It was noted that the off-centre distance of Li is higher than that of F. The QCCs of the charge transfer to and from C₆₀ were also analysed. Although charge transfer to and from the C₆₀ cage takes place in both cases, Li@C₆₀ becomes more polar than F@C₆₀, suggesting a better electron-accepting nature of C₆₀ than electron-donating behaviour. This fact is consistent with the natural bond orbital (NBO) charge on the trapped atoms and the dipole moment as well as the binding energy values of the encapsulated C₆₀. Although the encapsulation of both atoms reduces the frontier orbital energy gap, the frontier orbital gap of Li@C₆₀ is smaller than that of F@C₆₀. More interestingly, the depression in the polarizability of Li@C₆₀ is significantly large relative to that of F@C₆₀. These findings also support the tendency of C₆₀ to act as electron acceptor. This study provides some insights into the fundamental properties of C₆₀ and should be helpful in designing new endofullerene complexes for a variety of applications.

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Introduction

The most popular fullerene consists of 60 carbon atoms in the form of a hollow sphere, known as 'buckminsterfullerene' or a 'buckyball'. This was discovered by Smalley et al. in 1985,^[1] however, the structure was identified a few years earlier by Iijima from an electron microscope image.^[2] The hollow space enables fullerene to trap atoms or small molecules, and these were referred to as endohedral fullerenes or endofullerenes by Chai et al.^[3] Heath et al.^[4] discovered the first endohedral fullerene, La@C₆₀, by encapsulating an La atom inside C₆₀. Endohedral fullerenes have been interesting owing to their unique structures, novel electronic properties, and potential applications in a variety of fields, such as superconductors,^[5] optical switches^[6] solar cells,^[7] and nanotechnology, and biomedical applications.^[8] In the last few decades, many attempts have been made to dope C₆₀ using a variety of atoms and molecules^[9–17] because of their electronic structures, which might exhibit different spin configurations. Endohedral fullerenes are also interesting because they serve as precursors to potential new materials for nanotechnology and semiconductors and, therefore, many theoretical and experimental studies have aimed to discover as well as synthesize these novel nanomaterials.^[18–24]

Lithium (Li) and fluorine (F) are representative elements of the groups having the lowest ionization energy and highest electron affinity across the Periodic Table. Consequently, Li is more electropositive than C and F is more electronegative than C. Charge transfer takes place to and from C₆₀ when these atoms are trapped. Consequently, C₆₀ behaves as an electron acceptor in the case of Li@C₆₀ but an electron donor for F@C₆₀. The present work offers a comparative analysis of the various properties of Li@C₆₀ and F@C₆₀ using density functional theory (DFT). Many studies have been carried out on various aspects of Li@C₆₀^[25–30] but only a few on F@C₆₀.^[31,32] The objectives of the present study included whether C₆₀ is a better electron acceptor or electron donor. Further, we placed an emphasis on the changes in properties such as structural stability, and the vibrational and electronic properties of C₆₀ introduced by the trapping of Li and F atoms. We believe that this study provides better insights into the properties of endohedral fullerenes and should stimulate their possible applications.

Computational Methods

In the present work, we used the B3LYP functional with the 6-31G(d) basis set as implemented in *Gaussian 09*.^[33] B3LYP is

a three-parameter hybrid functional, which incorporates Becke's exchange term^[34] mixed with the HF exchange and correlation term of Lee, Yang, and Parr.^[35] The 6-31G(d) is a valence double-zeta polarized basis set in which six primitive Gaussian functions are used for core atomic orbitals, and valence orbitals are two basis functions comprising three and one primitive Gaussians. In addition, six *d*-type Cartesian-Gaussian polarization functions are included for each atom. The present computational scheme has already been found to be reliable in many previous studies on C₆₀ and related systems.^[36–39] Geometry optimization was performed without any symmetry constraint in the potential energy surface. The vibrational frequency calculations were performed at the same level of theory. The atomic charges were calculated using a natural bonding orbital (NBO) scheme^[40] as implemented in *Gaussian 09*.

Results and Discussion

The equilibrium structures of Li@C₆₀ and F@C₆₀ are displayed in Fig. 1. The bond lengths of Li@C₆₀ and F@C₆₀ along with those of C₆₀ are listed in Table 1. We can see that the length of the C–C bonds in the hexagon–hexagon (*d*_{H–H}) rings as well as hexagon–pentagon (*d*_{H–P}) rings are slightly elongated by encapsulation of the Li or F atom. In the case of Li@C₆₀, the Li atom is located close to the pentagon side at a distance of 1.52 Å from the centre of the C₆₀.

Li and Tománek^[27,28] already reported that the mean distance from the centre of Li inside C₆₀ was 1.5 Å, which agrees with the present calculations. In the case of F@C₆₀, the F atom is shifted and is 0.86 Å from the centre of C₆₀ cage. The equilibrium structures of Li@C₆₀ and F@C₆₀ were used to calculate their vibrational infrared spectra in the gas phase at the B3LYP/6-31G(d) level. For comparison, we also calculated the infrared spectrum of C₆₀ at the same level of theory. In order to assign the vibrational peaks, we analysed the graphical animation generated by the *Gaussview* program. Our vibrational analysis shows that all frequencies are positive for both Li@C₆₀ and F@C₆₀. This confirms that encapsulated C₆₀ belongs at the true minimum in the potential energy surface. We plotted the vibrational infrared spectra of Li@C₆₀ and F@C₆₀ along with C₆₀ in Fig. 2.

In C₆₀, we obtain four distinct peaks, two corresponding to two stretching (at 1460 and 1214 cm^{−1}) and bending (at 588 and 536 cm^{−1}) modes each. The encapsulation of the Li or F atom causes a modification in the intensity of the vibrational peaks due to change in the charge distribution and hence dipole moment. Note that the dipole moment of C₆₀ vanishes owing to its symmetry. However, Li@C₆₀ and F@C₆₀ possess non-zero dipole moments, 0.50 and 0.40 Debye (D) respectively (see Table 1), where 1 D is equal to the dipole moment of a pair of unit opposite charges situated at a distance of 0.208 Å. Therefore, vibrational peaks above 1500 cm^{−1} are obtained in both Li@C₆₀ and F@C₆₀. The intense peaks observed at 1366 cm^{−1} in Li@C₆₀ and 1222 cm^{−1} in F@C₆₀ correspond to the bending of ring atoms in the cage. The infrared intensity distribution clearly shows that more intense peaks are seen in the Li@C₆₀ than the F@C₆₀ system. This indicates that the Li@C₆₀ cage becomes more polar than F@C₆₀, consistent with their dipole moment values.

In order to analyse the charge transfer in encapsulated C₆₀, we computed NBO charges on the trapped atom (*Q*), as listed in Table 1. One can see that the charges *Q* on the Li and F atoms are +0.68 electron (*e*) and −0.40*e* respectively. A charge transfer of 30% from the Li atom to the C₆₀ cage has been previously

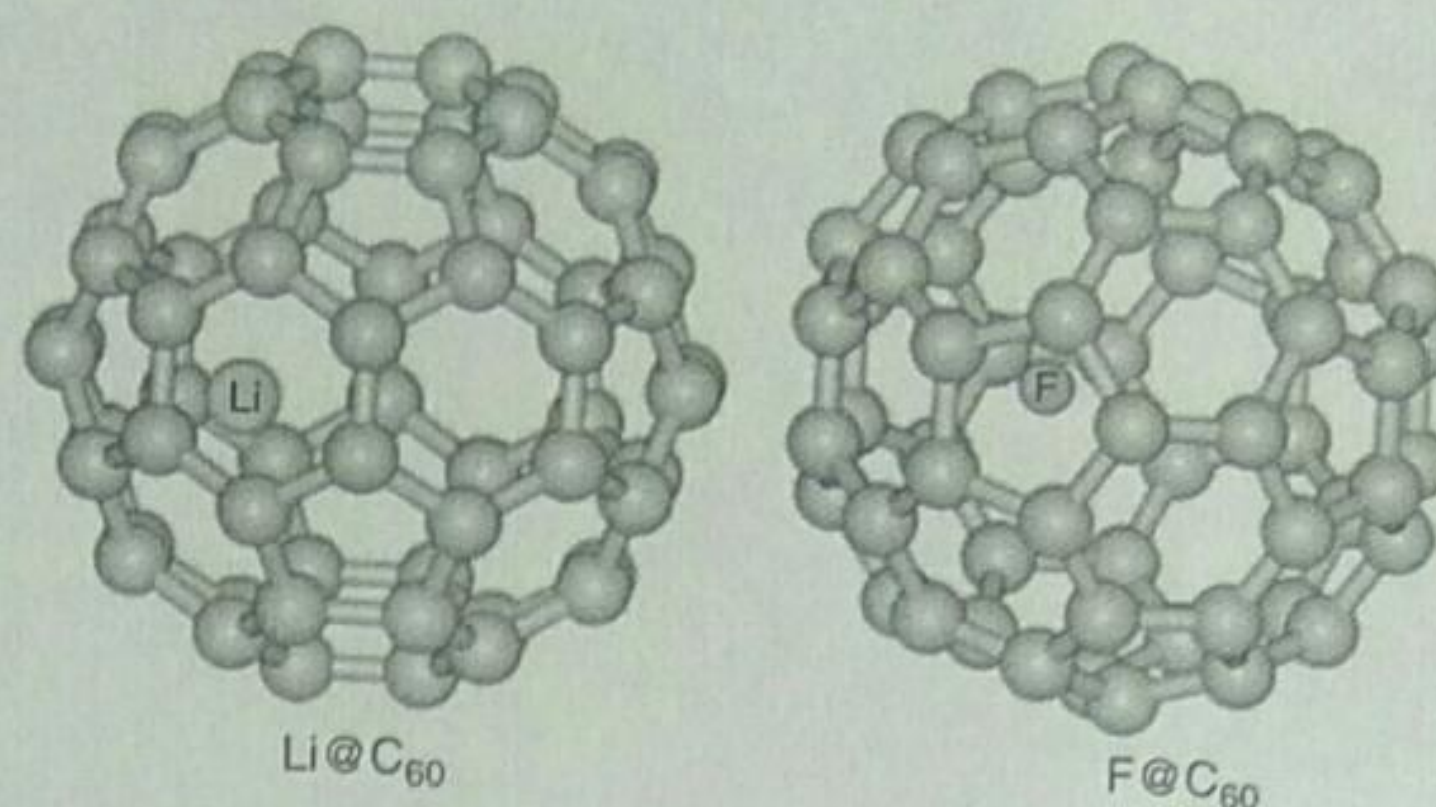


Fig. 1. Equilibrium structures of endohedral fullerenes considered in this study.

Table 1. Various parameters of Li@C₆₀, F@C₆₀ and C₆₀ calculated at the B3LYP/6-31G(d) level

Parameters		Li@C ₆₀	F@C ₆₀	C ₆₀
Bond lengths	<i>d</i> _{H–H} [Å]	1.40–1.41	1.40–1.41	1.40
	<i>d</i> _{H–P} [Å]	1.45–1.46	1.45–1.46	1.45
Distance from centre	<i>d</i> _{centre} [Å]	1.52	0.86	
Binding energy per atom	ΔE [eV] ^A	1.25	0.58	
NBO charge on trapped atom	<i>Q</i> [<i>e</i>]	0.68	−0.40	
Frontier orbital energy gap	<i>E</i> _{gap} [eV]	0.88	1.08	2.76
Dipole moment	μ [D]	0.50	0.40	0
Mean polarizability	α_o [au]	501.0	477.4	468.8
Depression in polarizability	$\Delta\alpha$ [au] ^B	−98.7	−6.9	

$$^A \Delta E = [60E\{C_{60}\} + E\{X\} - E\{X@C_{60}\}]/61.$$

$$^B \Delta\alpha = \alpha_o\{X@C_{60}\} - \alpha_o\{C_{60}\} - \alpha_o\{X\}.$$

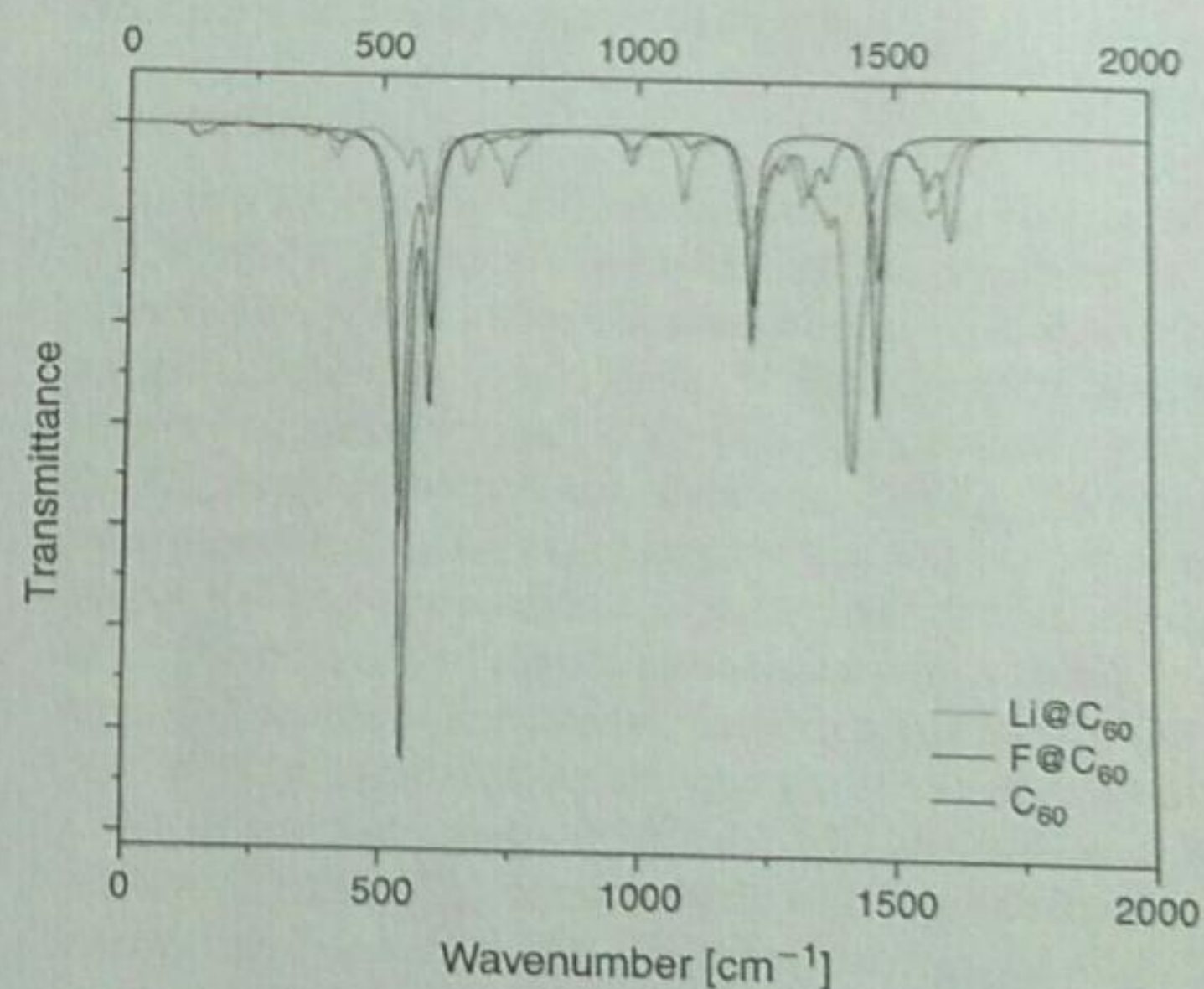


Fig. 2. Calculated vibrational infrared spectra of the systems considered in this study.

reported.^[27,28] Although the first ionization energy of Li is quite low and electron affinity of F is fairly high, the *Q* values are significantly smaller than unity. This may suggest the back-donation of charge within encapsulated C₆₀. For instance, there is back-donation of charge to Li from C₆₀ in Li@C₆₀ so as to reduce the net charge on Li to 0.68*e*. This was already noted in previous studies.^[17,37] In the case of F@C₆₀, in contrast, there is significant back-donation from F to C₆₀ such that the C atoms

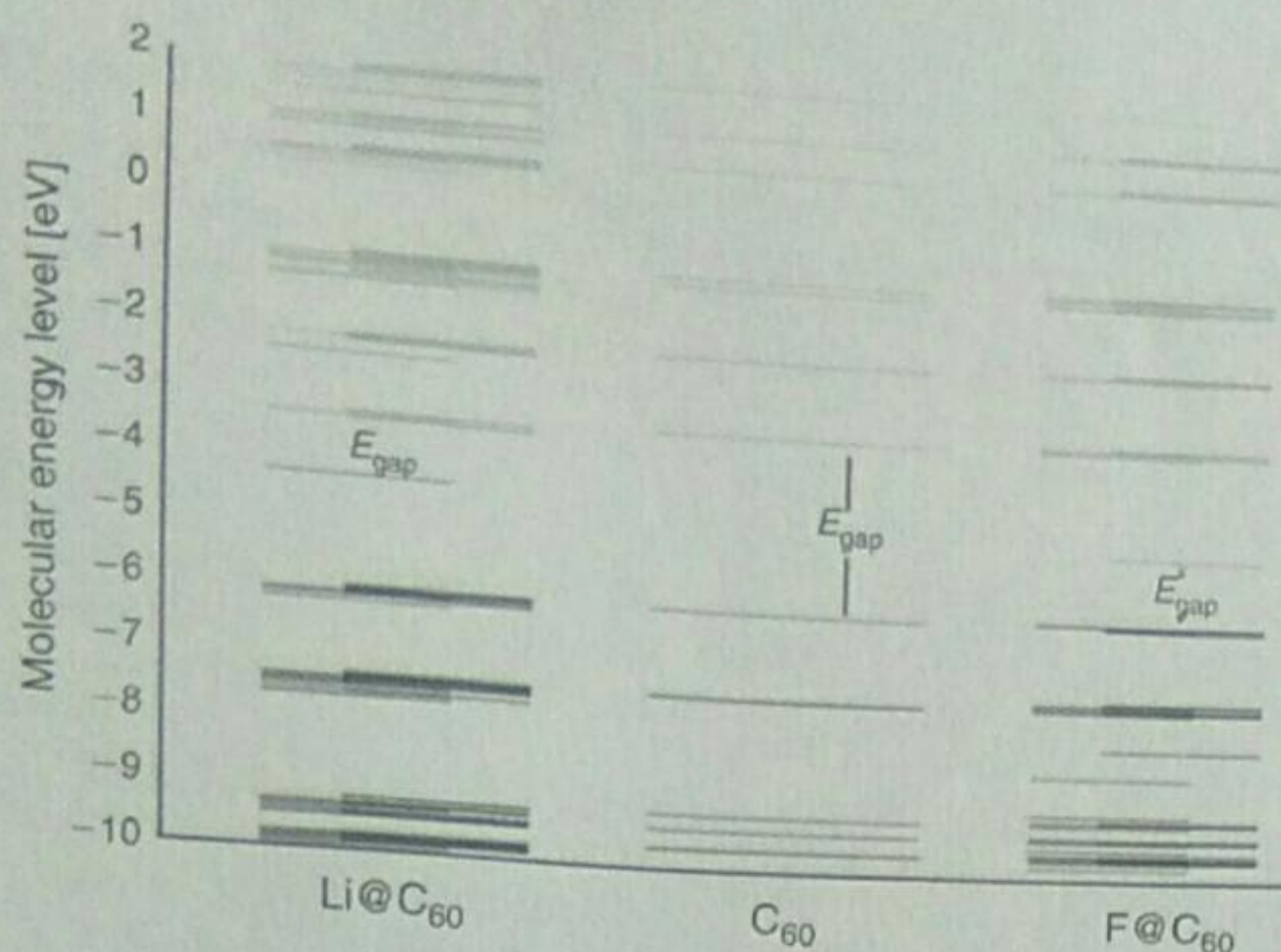


Fig. 3. Molecular orbital energy spectra of the systems considered in this study.

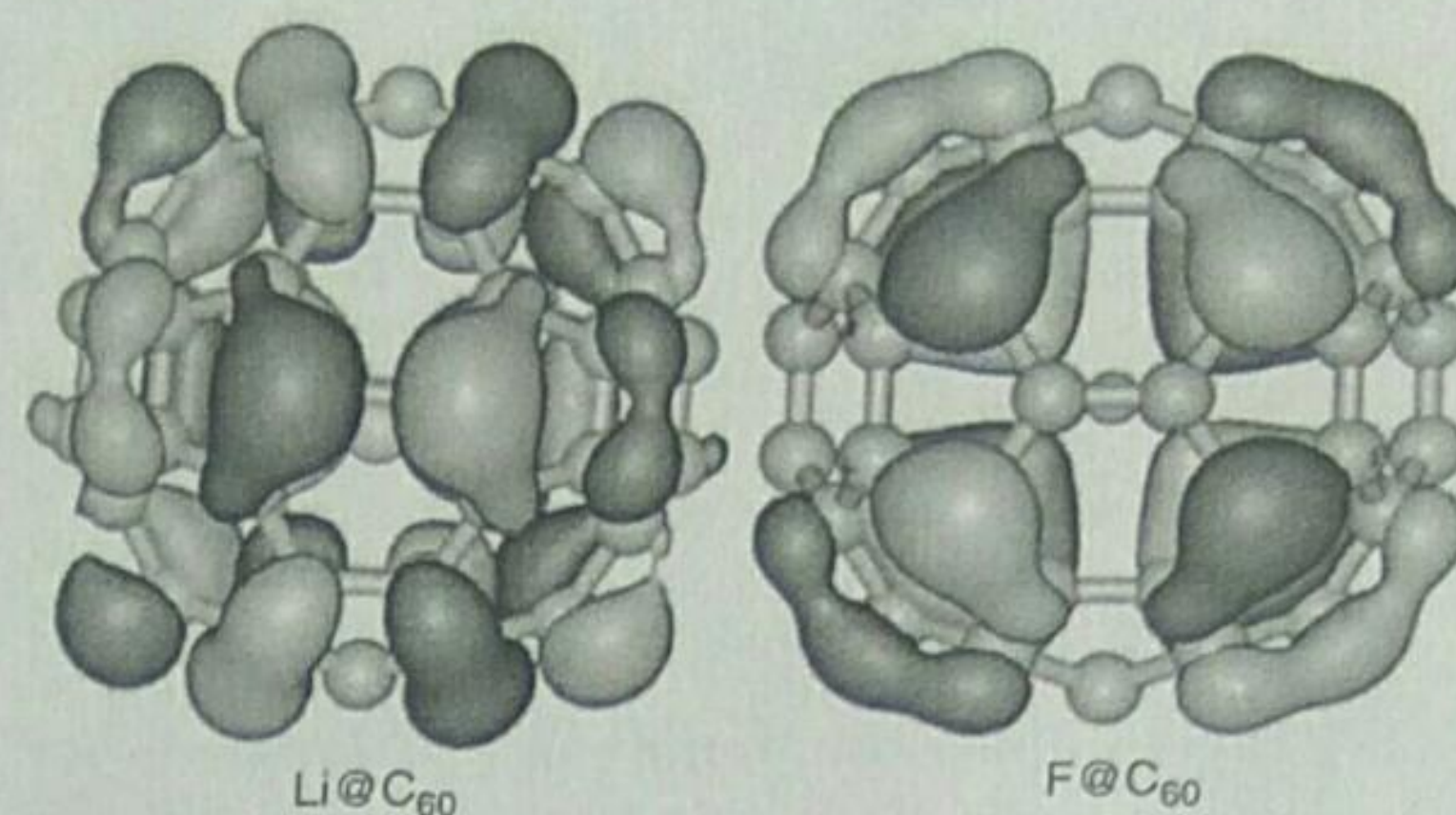


Fig. 4. The highest occupied molecular orbitals of endohedral fullerenes considered in this study.

become negatively charged (by $-0.003 e$) in the vicinity of the F atom. On comparing the charge transfer to and from C₆₀ in both cases, we notice that C₆₀ is a better electron acceptor than electron donor. This is clearly reflected in the dipole moment values of Li@C₆₀ and F@C₆₀ mentioned earlier. Furthermore, this fact is supported by the binding energy per atom (ΔE), listed in Table 1. Note that the ΔE of Li@C₆₀ (1.25 eV) is larger than that of F@C₆₀ (0.58 eV). This may suggest that C₆₀ becomes relatively more stable by accepting the charge from Li than by donating the charge to F.

The plotted molecular orbital energy level diagram of Li@C₆₀, F@C₆₀, and C₆₀ is shown in Fig. 3. The energy difference between frontier molecular orbitals such as the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) is referred to as the frontier orbital energy gap (E_{gap}), marked in Fig. 3. One can see that the E_{gap} value of C₆₀ is 2.76 eV, which decreases to 0.88 eV in Li@C₆₀ and 1.08 eV in F@C₆₀. This is possibly due to the fact that the encapsulation of Li or F introduces additional energy levels into the molecular orbital energy diagram. These additional energy levels tend to shift the HOMO energy up in Li@C₆₀ and the LUMO energy down in F@C₆₀, consequently reducing the energy gap. In Fig. 4, we show the HOMO surfaces of Li@C₆₀ and F@C₆₀. In both cases, the HOMO is contributed by C atoms of the cage. However, the major contribution comes from C atoms in the vicinity of Li in the case of Li@C₆₀ but C atoms far away in the case of F@C₆₀.

As encapsulated C₆₀ becomes polar owing to charge transfer to and from the Li or F atom, we calculated the mean polarizability (α_0) of Li@C₆₀ and F@C₆₀, also listed in Table 1. The components of polarizability are computed by numerical differentiation using a uniform electric field of magnitude 0.001 atomic unit (au). The α_0 of the empty C₆₀ cage, Li, and F atoms are 468.8 au ($\approx 70 \times 10^{-24} \text{ cm}^3$), 130.9 au ($19.37 \times 10^{-24} \text{ cm}^3$), and 1.67 au ($0.25 \times 10^{-24} \text{ cm}^3$) respectively, which agree well with the corresponding experimental values^[41] of 76.5×10^{-24} , 24.33×10^{-24} , and $0.55 \times 10^{-24} \text{ cm}^3$ respectively. For encapsulated C₆₀, α_0 increases compared with empty C₆₀ owing to charge transfer within the cage. In order to analyse the effect of the trapped atom on polarizability, we computed the depression in polarizability ($\Delta\alpha$). For Li@C₆₀, $\Delta\alpha < 0$, i.e. a depression of polarizability takes place (see Table 1). It has been already reported^[42] that the encapsulated

metal atom inside larger fullerenes such as C₆₀ is compressed and the total polarizability decreases. However, this depression is very small in the case of F@C₆₀ owing to the smaller magnitude of $\Delta\alpha$, 6.9 au relative to 98.7 au in Li@C₆₀. According to the model of quenched polarizability,^[43] the polarizability of C₆₀ does not change significantly on encapsulation of atoms (molecules). Therefore, $\Delta\alpha$ is related to the decrease in polarizability of encapsulated atoms (molecules). Thus, the effect of encapsulation is stronger on Li atom than F atoms, as far as C₆₀ is concerned. This fact also agrees with the aforementioned properties of Li@C₆₀ and F@C₆₀. The theoretical results such as the HOMO–LUMO energy gap, dipole moment, and polarizability discussed here may be useful in the design of charge-transfer complexes consisting of Li@C₆₀ and F@C₆₀ systems. Such complexes are likely to possess strong non-linear optical properties. Further work in this direction is in progress in our laboratory, and will be reported shortly.

Conclusions

A comparative study on Li@C₆₀ and F@C₆₀ performed at the B3LYP/6-31G(d) level revealed that the structure of C₆₀ is equally affected by either encapsulation of Li or F, producing a marginal difference in bond lengths. The off-centre distance of F is, however, smaller than Li. There is charge transfer to and from the C₆₀ cage in both cases, although Li@C₆₀ becomes more polar than F@C₆₀. This may suggest that C₆₀ is a better electron acceptor than electron donor. This fact was further supported by the NBO charge and dipole moment as well as binding energy values. The molecular orbital analysis suggests that the encapsulation results in shifting the energy of the HOMO higher in Li@C₆₀ and the energy of the LUMO in F@C₆₀ is lowered relative to empty C₆₀, consequently reducing the frontier orbital energy gap, reducing the ionization energy of Li@C₆₀, and increasing the electron affinity of F@C₆₀. We also noted that the effect of encapsulation on polarizability is only marginal in the case of F@C₆₀ but that of Li@C₆₀ is strongly affected. These findings may be useful in the design of new systems based on these prototype endohedral fullerenes.

Supplementary Material

The Cartesian coordinates of C₆₀ molecule and Li@C₆₀ and F@C₆₀ complexes are available on the Journal's website.

Conflicts of Interest

The authors declare no conflicts of interest.

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Climate Change and Traditional Method of Rain-Water Harvesting in Magadh Plain

Dr. Kuntal Kishor

Climate change and its impact on geo-hydrological characteristics of land is a matter of concern for most of the world. Large numbers of projects and researches have been carried out by government and non-government organizations to find out the possible impact of climate change on availability of water. In view of changing geo-hydrological characteristics of lithosphere there is need of sustainable source of water. This study is aimed to find out the sustainability and reliability of traditional methods of rain water harvesting and use of harvested water for irrigation in Magadh region. Data and information collected from different secondary sources have been analyzed to find out the sustainability of these traditional methods. Since ancient times Ahar-Pyne system, Ponds and Tanks have been used in the study area for collection of rain and flood water and its distribution for irrigation purpose. Traditional methods of rain water harvesting have been found suitable for the study area as it is based on local geomorphic and climatic conditions. These methods are more sustainable and useful than modern methods of rain and flood water collection and distribution. Water harvested through these methods can be used for irrigation purpose during dry season and during failure of monsoon. It also helps in recharging of underground aquifers.

Key Words : Climate change, Geo-hydrological, Lithosphere, Sustainable, Rainwater harvesting, Ahar-Pyne, Monsoon, Aquifer.

Introduction : The human induced changes in climatic conditions have now gained a wide scale focus of the intellectuals and the governments all over the world. Environment scientists and Climate experts have not only warned us against the possible negative effects of climate change but also provided us the suggestions and the measures to be taken to get rid of it or to reduce its impact. It has now become a subject matter of almost all disciplines, such as: environmental science, environmental management, geography, earth science, urban and regional planning, meteorology, biogeography etc. One of the most disastrous effects of climate change is change in hydrological cycle and consequent changes in precipitation patterns and extremes of climate (cyclone, tornado). With the increase in population, industrial development and green revolution demand of water has increased voluminously for domestic, industrial and agricultural purposes. The ground water and surface water resources have been exploited without proper care and above the rate of replenishment. So, now pure water resource has become one of the scarce resources on earth. There is urgent need to replenish and conserve pure water for sustainable growth of human being. India lies in tropical belt and get most of her precipitation in the form of rainfall, so the rainwater need to be harvested as it flow down the slope towards the streams and drains, and ultimately reaches to the ocean without used. In higher latitude region precipitation is in the form of snow which does not flow quickly down the slope and thus, melt water slowly percolate to the underground aquifers.

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Climate change refers to the change in average weather conditions of any area that has been a characteristic feature of that area for a long period of time. This shift from average conditions of weather may be induced by natural as well as anthropogenic causes. The last phase of natural climate change was witnessed during little ice age (14th century A.D.). The present discussion about the climate change is anthropogenic in nature. Industrial development and effluence of large scale pollutants, sizeable growth in population, decline in forest cover has resulted in increase in global average temperature due to green house effect and ozone depletion. It has further increased the concentration of carbon dioxide and Methane gas from thawing permafrost and warming ocean. Thus a cycle of increase in carbon dioxide concentration has begun. The chaos of global warming and disturbance in hydrological cycle has forced us to reconsider the sustainability of our present day water management techniques and to reintroduce the area based (ancient approach) of water harvesting based on long experience of local climatic and geo-hydrological conditions. This research paper tends to provide the assessment of ancient techniques used in Magadha plain for rain water harvesting and measures taken by the government and non-government organizations for its development.

Present study is focused on the methods adopted for water harvesting in Magadh plain since ancient times. The study area is situated in south-western part of Bihar. The plain is situated south of river Ganga, east of river Son, west of Anga plain and north of Peninsular plateau.

Objective : The main objective of the study is to assess the traditional method of rain water harvesting in the Magadh plain and its applicability in present circumstances. This study is also aimed to find out sustainability of these techniques in stipulation of changing precipitation pattern, failure of monsoon and geo-hydrological characteristics of study area. Researchers also tried to find out the historical development of these methods and social and technical conditions that assist its viability.

Methodology : Present study is based on analytical description of information gathered from different secondary sources. The study is historical in nature as it tends to explain the evolution and development of traditional water harvesting system, and it is idiographic in sense that it tends to provide the analytical description of the situation of water harvesting methods, sustainability of traditional method of rain and flood water harvesting and changing trend of water utilization habits.

Geological Structure and Hydrological Characteristics of Magadha Plain : The Magadha plain is surrounded by river Ganga in north, Son-Ganga divide in west, Anga plain in east and peninsular plateau in south. The predominant geological formations in Magadha plain are: mica schist, amphibolites, quartzite, granite dolerite and pegmatite of Proterozoic period, and gneisses, granite, phyllite of Archean period (in form of peninsular outgrowth) together with alluvial deposits of Ganga, Son, Falgu, Niranjana and its tributaries (Holocene period). The Vindhyan in Bihar are exposed in Rohtas and Bhabhua districts as scarp and plateau. The soils found in Magadha plain are: Sand, clay red and yellow, alluvial, and mixture of sorted gravels and sand, and of sand and clay.

The Magadha plain is drained by many rivers like Son, Falgu, Niranjana, Karmanasa, Durgawati, Dhamuti, Punpun, Morhar, Dardha, Paimar, Dhadhar, Sakri, Badua and Chandan. The average gradient of one meter per kilometer towards north and northeast in Magadha plain pushes the water from Rohtas and Chhotanagpur plateau towards river Ganga. This slope is the main driving force behind not only the major natural river system but also for canal and *Ahar-Pyne* irrigation system. The region gets average annual rainfall of 110 cm

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mainly during south west monsoon season. The failure of monsoon predicts the decrease in food crop production in the area, as most of the river and canal are rain fed and get less water during weaker monsoon.

The water bearing rock systems in the region are weathered and fractured granite rock and alluvium. The water bearing formation can be divided into

- Fissured formations-** These are characterized by presence of fissure in rock strata or newly weathered parental rock. The ground Water is found in these fracture zones or in spaces between two rocks. The thickness of this formation is 2-10 meter in high ground and 10-15 meter in low lying area. The boreholes drilled by Central Ground Water Board (CGWB) in the hard rock terrain have tapped fractures at variable depth from 14-98 meter.
- Porous formation-** The Quaternary alluvium of river valleys constitutes this hydro geological unit. It consists of alluvial sediments made up of gravels, sands, silt and clays. The gravel and medium to coarse-grained sand layers are good groundwater repositories. The thickness of the alluvium deposit is nearly 30-50 meter.

Water Utilization Habits and Sources of Water : The whole population of Magadha plain depends on groundwater for their drinking need except few urban areas which get the water supply from nearby rivers. A part of the drinking need of towns in Magadh Plain is met from the Rivers due to lack of any potential aquifer beneath the towns. For agricultural and industrial use people depend on underground water, canal and other surface water reservoirs (Table-1).

Table-1
Total irrigated area through different sources in Magadh region

Districts	Canal	Tube well	Other sources	Total irrigated area
Patna	51115	121049	7431	179595
Nalanda	9442	164270	19576	193288
Bhojpur	40781	135775	11538	188094
Buxar	44421	66410	3079	113910
Rohtas	262570	36037	32227	330834
Kaimur	98493	54414	13630	166537
Gaya	232303	-	2787	235090
Jehanabd	596	57839	8771	67206
Arwal	28712	18034	1385	48131
Nawada	13944	108831	3783	126558
Aurangabad	142664	65794	15743	224201
Total	925041 (49.38% of total irrigated area)	828453 (44.22% of total irrigated area)	119950 (6.4% of total irrigated area)	1873444

Source: Central Water Commission, Dept. of Water Resources, Bihar and Central Ground Water Board.

Farmers of Magadh region use pump set to fetch water from rivers and pond, and bore well to tap underground water for irrigation purpose. East and west Son canal is one of the main sources of irrigation in canal command area. For domestic use underground water is tapped through hand pump and bore well. Earlier, people used to depend on dug well to tap

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groundwater for domestic purpose. For irrigation and industrial purpose people used to use Ahar- Pyne, Pond, River and Dug well. Potential sources of water in the region have been ground water, rivers and ponds.

Traditional Methods of Rain Water Harvesting In Magadh Plain : "In scientific terms, water harvesting refers to collection and storage of rainwater and also other activities aimed at harvesting surface and groundwater, prevention of losses through evaporation and seepage and all other hydrological studies and engineering inventions, aimed at conservation and efficient utilization of the limited water endowment of physiographic unit such as a watershed." The traditional methods of rain water harvesting that existed century ago in various states of India are relevant today as it is based on local conditions and are perhaps even more useful than the modern water harvesting techniques. These traditional methods of rain water harvesting were not only based on experience of local geo-hydrological conditions but also fitted to the long developed social mosaics. So, for the sustainable collection and utilization of rain water traditional methods are more useful than the modern one. *Ahar-Pyne, pokhar and well* are some traditional techniques used for rain water harvesting in the study area. Among these, *Ahar-Pyne* system is most successful and sustainable method of rain water harvesting and irrigation in Magadh region.

Ahar and Pyne : Agriculture practices developed in Magadh plain about 4000 years ago. *Ahar-Pyne* system was developed by the local farmers to have perennial access to water for irrigation. When, sufficient amount of water is not provided the productivity of crop decreases. During rainy season the area get 110 cm of rainfall and water from over flooding river and top rocky region flow down the slope. *Pyne*, a narrow man made channels running down the slope from base of a hill, river or pond collect over flowing water and ultimately ends in to an *Ahar* (a reservoir having embankment on three sides) [Figure-1].

Table-2 : Area irrigated by Ahar and Pyne system

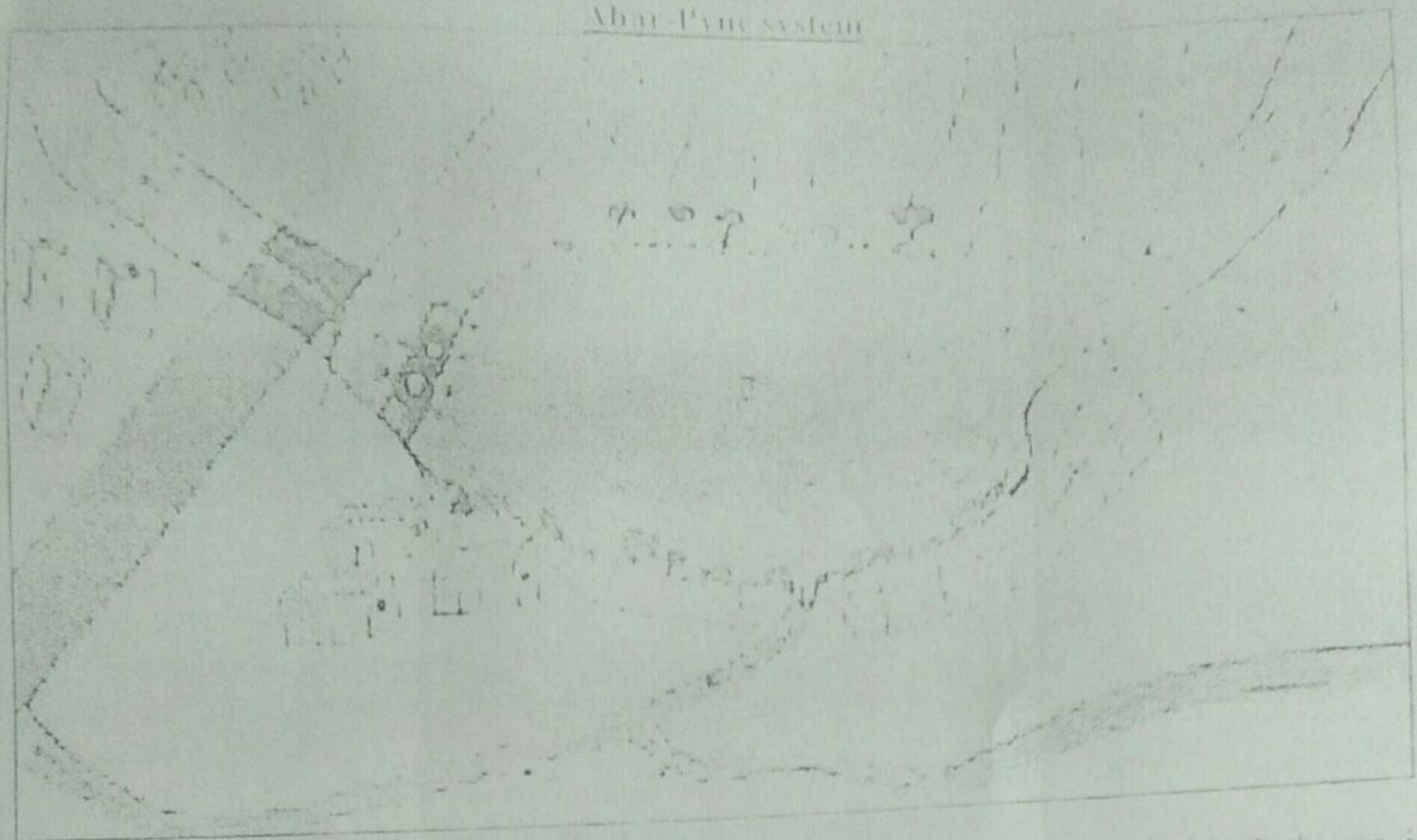
year	Area irrigated (mha)	Region covered
1930	0.94	South Bihar
1971	0.64	South Bihar
1976	0.55	South Bihar
1997	0.53	Whole of Bihar

Source: http://www.indiana.edu/~iascp/Final_pant.pdf.

Large network of *Ahar* and *Pyne* were developed during Mauryan and Nanda period and since then it has been used for rain and flood water harvesting. It was this irrigation system that allowed the farmer of Nalanda to feed more than 10000 students and 1000 teachers of ancient Nalanda University. Rivers like Punpun, Sone, Ganga, Morhar, Lilajan, Mohane, Phalgu, Dhadhar, Mangura, Jakori, Tilaiya, Khuri, Dhanarji, Sakari, Nata, Baghel, niranjana etc. supported this system of water harvesting. It loosed its importance partially due to development of modern canal irrigation system, tube well and bore well, pump set and mainly due to disorganization of social institutions set up for construction and maintenance of *Ahar* and *Pyne*. Since the introduction of new irrigation techniques by British and its continuous development during post-independence phase this method of rainwater harvesting losing its importance (Table-2). Some NGOs like DHAN foundation, Satyapath and Magadh Jal Jamaat have shown keen interest in rejuvenation of this system of rain water harvesting during recent past.

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Figure 1
Ahar-Pyne system



Source: rainwaterharvesting.org

Sustainability of ahar-pyne system : In view of uncertainty of monsoon and change in climatic conditions it has been advised by the scholars that there is need of sustainable development of agriculture to feed our rapidly growing population. Sustainable development of agriculture demands for sustainable source of irrigation. Modern developed techniques such as tube well, bore well deplete the underground water and water table is gradually going down year by year. Further canals are not a perennial source of water in Magadh region. On the other hand ahar-pyne is best suitable method for rain water harvesting, recharge of underground aquifers and irrigation. In this region slope of ground is favorable for development of ahar-pyne which collect rain and flood water for irrigation. Some part of water collected in ahar percolate down the ground and recharge aquifers and rest are used for irrigation in dry season or during failure of monsoon. So it is sustainable and most suitable method of rain water harvesting in the study area developed by local farmers on the basis of their long experience of local geomorphic and climatic conditions

Other Methods : Flood and rainwater move down the slope and collected in manmade or natural depression, we name it pond, tank or lake. The water harvested in ponds and tanks have been used by local farmers since ancient times. There were large number of tanks (in hilly region) and ponds (in plain) in the study area. But negligence and unavailability of proper maintenance of these reservoir most of them became plain and dry due to siltation. Some remaining ponds are still used by farmers for irrigation purpose. There is large pressure of population on these water bodies and they cannot meet the needs of local farmers. If these ponds and tanks are rejuvenated it can hold water for dry season and underground aquifers will also be recharged.

Conclusion : Recent changes in precipitation pattern due to climate change, drying surface water sources and depleting underground water due to non-replenishable excessive use of these water sources are some serious concerns for farmers, scholars and the governing bodies

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in the study area. There is an urgent need to make efforts to provide sustainable source of irrigation to farmers and to recharge underground aquifers for growth of flora and fauna. Problem of water shortage in the region can be sorted out by rejuvenation of ahar and pyne system, ponds and tanks. These surface water sources are not only the back up for water needs during dry season but also help in recharging underground aquifers. Further, these water sources were developed by local farmers in accordance with the local climatic and geomorphic characteristics. So these are sustainable and reliable sources of water which needs less investment than development of canals and dams.

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S. B. Poddar

Geography of Crime against Women in Metropolitan India

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Spatial variation in rate of crime against women predicts the spatial pattern of women empowerment and social health in different geographical area. This study tries to find out the spatial variation in crime against women in metropolitan cities of India having population above two million. It also incorporates the possible cause of this spatial variation. To know the spatial variation in crime against women, data and information has been collected from National Crime Record Bureau (NCRB) report of 2016, newspapers and journals. Data collected from secondary sources after statistical and descriptive analysis reveals the spatial variation in rate of different crimes against women. This study incorporates statistical, descriptive, comparative and analytical study of data related to crime against women in metropolitan cities of India which suggests that: Metro cities in north India register highest rate of crime against women followed by metro cities of central and south India, some crimes are more common in particular area. The possible causes for this spatial variation have also been briefly discussed in this paper. Therefore this study is an attempt to know the spatial variation in rate of crimes committed to women and the possible cause behind it.

Key Words: Spatial variation, Spatial pattern, Women empowerment, Social health, Statistical, Descriptive, Comparative, Analytical

Introduction : Crime against women in India is one of the least studied common phenomena. Since the advent of great human civilizations women played an important role in the development of society. Gifted with motherhood they nurtured the mankind to their optimum level of development but unfortunately crime against women has been the part of society since the beginning. Women in ancient India enjoyed respectable place in their societies but today women are easy prey for criminals and even family members. Male dominated social, economic, legal and political order (Atray 1998; Verma 1990; Nagla 1993 and Mukherjee 2001), activities for political gains (Karat, 1998), increasing participation of women in socio-economic, administrative and political system (Rajan 1981; Deshpande 1984 and Ganguli 1990) make women vulnerable to crime. In year 2016, 29 lakh FIRs were registered in India. Crimes against women contribute to about 10% of all crimes (Economic Times, Nov. 24, 2018). The recorded data of crime against women do not represent the actual number of incidents of crime against women in India. National Family Health Survey (2016) shows that less than 0.1% women who were victim of sexual violence went to the police. Crime victimization survey to know dark figure (Biderman, 1991) conducted in Rajasthan shows that only 29% of victims go to the police station and only 19% victims register case (Banerjee, Chattopadhyay, Duflo, Kensiton and Singh, 2012). So change in recent data regarding number of crime against women may be due to the change in reporting of crime. The rate of reporting of crime against women in metropolitan India is relatively higher than in rural areas. National Crime Record Bureau is a nodal agency that prepares report of different types of crimes including crimes against women in India on the basis of FIRs and complaints

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in different police stations. Total 41,761 cases of crime against women registered in Metropolitan cities (having population more than 2 million) of India in 2016. It is 5.16% of total crime committed in these Metropolitan cities (Crime in India 2016 statistics, NCRB, Ministry of Home Affairs). Low percentage of crime against women is only due to reasons associated with social stigma, malfunctioning of legal system and fear of retaliation (Mukherjee, Rustagi and Krishnaji, 2001). If proper reporting were done it would have increased up to 50% in Metropolitan India.

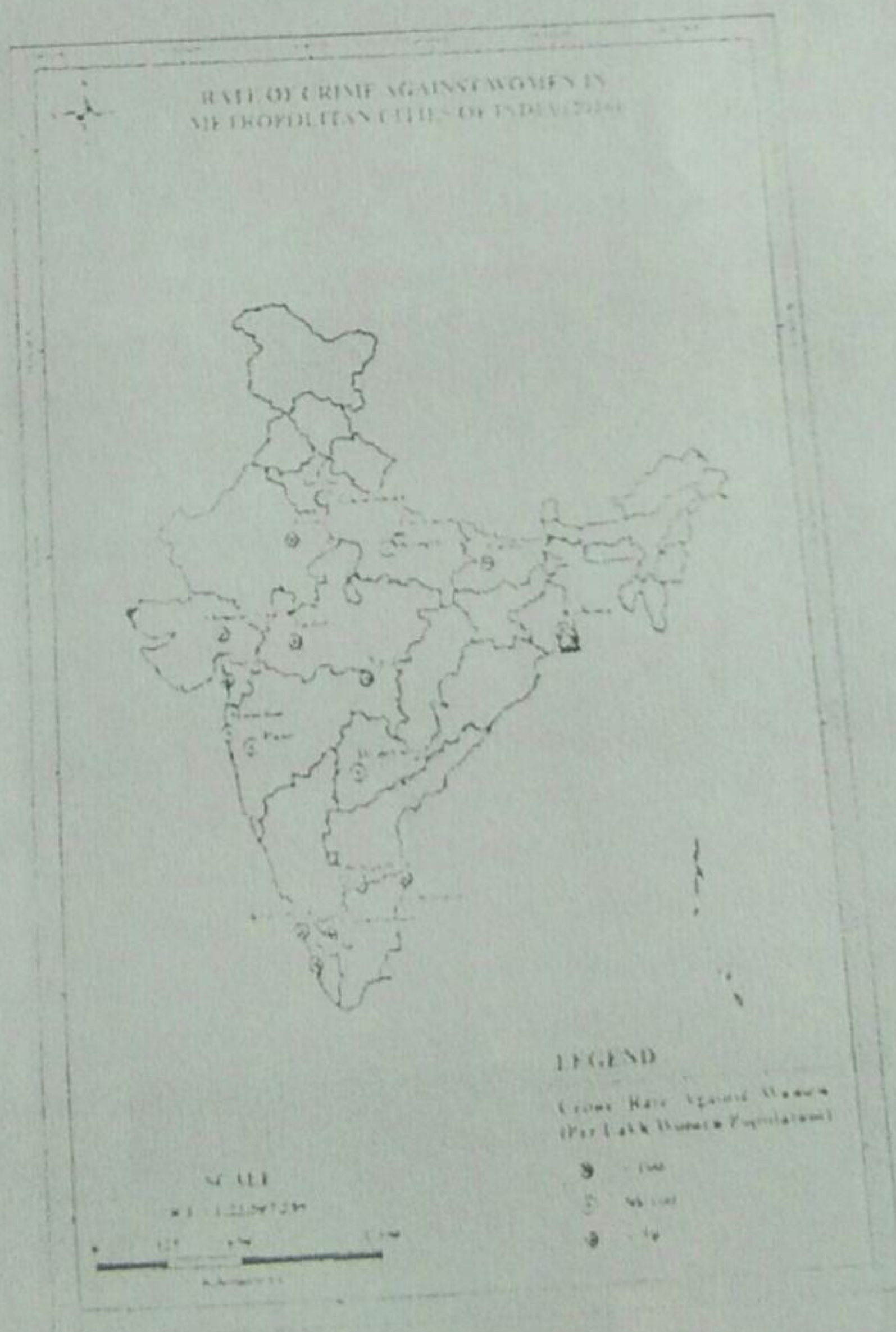
Objective and methodology : The main objective of this paper is to find out the spatial pattern of crime against women in metropolitan cities of India. For this purpose data has been collected from National Crime Record Bureau report (2016). These data has been analyzed to find out the spatial pattern, if any, of crime against women in big cities of India. Spatial pattern of intensity of different crimes against women have been calculated on the basis of averaged rank score of metro cities of north, central and south India. Averaged rank score for different crimes has been calculated by average of ranks of concerned towns in different parts of India (north, central and south). The city with highest crime rate has been given rank one, and so on. Cities with same crime rate have been given same rank. The crime rate in this paper has been calculated as number of crime against women per one lakh women population. Region with low averaged rank score has highest intensity of crime and region with high averaged rank score has low intensity of crime. In this paper author has used descriptive, comparative and analytical approach to describe crime against women, its spatial pattern and spatial variation in metropolitan India.

Crime against women in India: statistical overview : In 2016 out of total 4831515 numbers of crimes reported in India 338954 crimes were committed to women. So, only 7% of reported crimes in India were committed against women. Rate of crime against women in India is only 55.2 (per lakh of women) which is 379.3 (per lakh population) for whole population of India (NCRB report 2016). The reported data of crimes shows that crime rate against women is significantly lower than the overall crime rate in India. But the actual picture is different from the statistical facts due to dark figure (Biderman, 1991). Rate of crime against women in twenty nine states of India is only 53.6. It is 137.6 for seven union territories of India.

Crime against women in metropolitan cities of India: statistical overview : Metropolitan cities have population above one million. There are 53 million cities in India (Census, 2011). Out of which 19 cities have population above 2 million. Metro cities with 2 million population are area of study in this research paper. It include, Delhi, Ghaziabad, Jaipur, Kanpur, Kolkata, Lucknow and Patna from northern India, Ahmedabad, Indore, Nagpur and Surat from central India, and Bengaluru, Chennai, Coimbatore, Hyderabad, Kochi, Kozhikode, Mumbai and Pune from southern India. Out of these nineteen metropolitan cities, Maharashtra and Uttarpradesh occupy three cities, Gujarat, Tamilnadu and Kerala occupy two cities, and Karnataka, Telangana, Madhyapradesh, Rajasthan, West Bengal, Bihar and union territory of Delhi occupy one city.

Average crime rate in cities having population above two million is 709.1. Highest crime rate among these nineteen cities has been found in Kochi (2553.1) followed by Nagpur (1714.6), Chennai (1308.6), Delhi (1263.9) and Surat (1243.3). Other metropolitan cities have crime rate less than 1000 per lakh population. Average rate of crime against women in the study area has been found 77.2. Highest rate of crime against women has been found in Delhi (182.1) followed by Lucknow (159.8), Jaipur (144.1), Patna (133.8), Nagpur (113) and Indore (101.4). In other thirteen metro cities rate of crime against women is below 100 per lakh

women population. Rate of crime against women is lowest for Coimbatore (9.5) followed by Chennai (12.6), Kolkata (24.9) and Surat (28.7). If we calculate averaged rank score for metropolitan cities in northern, central and southern India on the basis of crime rate (Table-1) we find that metro cities in central India have highest intensity of crime followed by metro cities of northern and southern India respectively. Averaged rank score for crime in Northern India = $\text{Sum of rank (on the basis of crime rate) of cities in Northern India} \div \text{Total number of metro cities in Northern India}$. So averaged rank score for metro cities in northern India = $(4+12+6+17+19+10+8) \div 7 = 10.86$. Similarly it is 10.63 for metro cities in Southern India and 7.25 for metro cities in Central India. Lower averaged rank score for crime in Central Indian metro cities means, high intensity of crime in these cities. Spatial pattern of rate of crime against women is different from the pattern for overall crime rate. Averaged rank score for rate of crime against women in north Indian metro cities is 6.286. It is 10 for central Indian metro cities and 13.25 for metro cities of southern India. On the basis of this we can conclude that as we move northward in India intensity of crime against women in metro cities increases. Out of total crimes in nineteen metropolitan cities concerned for this study, only 5.16% crime is committed against women. In Hyderabad 13.22% of total crime is committed to women. It is followed by Lucknow (11.69%), Kanpur (11.32%), Pune (10.90%), Mumbai (8.68%), Ghaziabad (8.24%), Patna (7.66%), Bengaluru (6.96%), Jaipur (6.86%), Kolkata (6.78%), Delhi (6.70%), Indore (6.40%), Ahmedabad (3.55%), Nagpur (3.22%), Kozhikode (2.01%), Coimbatore (1.00%), Surat (0.99%), Kochi (0.72%) and Chennai (0.48%). National average for crime against women out of total crime is 7%



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Types of crime against women in metropolitan India : The nature and intensity of crime against women in India have changed over time. Ancient Indian society was ideal in which women enjoyed respectable place. In medieval age several social ills (*sati pratha, dand*) paralyzed the equal status and freedom of women in India. Though, rejuvenation of Indian social system by different social activists during British period, legal action against anti-social and unethical practices by governments together with increased participation of women in socio-economic, administrative, academic and political system has considerably changed the status of women in postmodern society. But rate of crime against women is still increasing every year. Different types of crime committed against women in metropolitan cities of India has been classified by Indian Penal Code (IPC) as: Dowry death (Sec. 304, IPC), Abetment of suicide of women (Sec. 306, IPC), Causing miscarriage without women's consent (Sec. 313, IPC), Acid attack or attempt of acid attack (Sec. 326 A or B, IPC), Cruelty by husband or his relatives (Sec. 498, IPC), Kidnapping and abduction of women (Sec. 363 to 369, IPC), Human trafficking (Sec. 370, IPC), Rape or attempt of Rape (Sec. 376, IPC), Unnatural offences (Sec. 377, IPC), Assault on women with intent to outrage her modesty (Sec. 354, IPC) and Insult to modesty of women (Sec. 509, IPC). Among these crimes in metropolitan India, rate of crime is highest for cruelty by husband or his relatives (22.6) followed by assault on women with intent to outrage her modesty (19.3), kidnapping and abduction of women (17.1), rape or attempt of rape (9.4), insult to modesty of women (3.5), dowry death (0.9), abetment of suicide of women (0.7), unnatural offences (0.2), causing miscarriage without women consent (0.2), acid attack or attempt of acid attack (0.1), and human trafficking (0.1).

Cruelty by husband or his relatives : It is the most common crime in metropolitan cities of India with the rate of 22.6 incidences per lakh of women population. Highest rate of crime associated with cruelty by husband or his relatives has been observed in Jaipur (69.5) followed by Lucknow (64.9), Delhi (48.1) and Ghaziabad (43.7). In Coimbatore (3.5), Chennai (4.1), Mumbai (6.9) and Surat (9.9) [Table-2] rate of incidence of cruelty by husband or his relatives is relatively lower. The averaged rank score for this crime in metropolitan cities of north, central and south India are 5, 10.75 and 14. It means, incidences of cruelty by husband or his relatives is most common in metropolitan cities of north India followed by central and south Indian metro cities. The main reason behind this spatial difference is lower women empowerment in northern India followed by central and southern India, and high unemployment rate in metro cities of northern and central India (Hindustan Times, 6 April 2017).

Assault on women with intent to outrage her modesty : It is the second most common crime against women of metropolitan cities in India. Rate of incidence of assault on women with intent to outrage her modesty in metropolitan cities of India is 19.3 per lakh women population. Delhi (49.4), Nagpur (33.7), Lucknow (29.9) and Pune (27.7) have high rate for this crime on the other hand Chennai (1.5), Coimbatore (1.8), Surat (2.8) and Ahmedabad (4.4) have low rate of incidence of assault on women with intent to outrage her modesty (Table-2). Averaged rank score for metro cities of north, central and south India are 8.14, 9.75 and 11 respectively. Therefore, as we move northward intensity of incidence of this crime increases in metro cities of India. The main reason behind this spatial difference is high rate of unemployment in metropolitan cities of north and central India and poor social status of women in these cities (Mukherjee, Rustagi and Krishnaji, 2001).

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Abetment of suicide of women : Abetment to commit suicide by women is one of the most uncommon crimes in metro cities of India. The rate of this crime is only 6.7 incidences per one lakh women population in concerned cities. Nagpur (2.6), Jaipur (2.4), Bengaluru (1.9) and Pune (1.6) are some of the cities where rate of abetment of suicide of women is relatively high. On the other hand it is nil (0) for Coimbatore, Ghaziabad, Kochi, Kozhikode, Lucknow and Patna (Table-2). Averaged rank score for this crime in metropolitan cities of north India is 8.7. It is 4.5 and 7.1 respectively for metro cities of north, central and south India. So, central Indian metro cities have higher intensity of this criminal activity followed by metro cities of south and north India. Higher intensity of abetment of suicide by women in metro cities of south and central India is due to changing social order in advanced societies of India and mental pressure by the abettor.

Other crimes against women : Unnatural offences and causing miscarriage without women consent (0.2 per one lakh women population), and acid attack or attempt of acid attack and human trafficking (0.1 per one lakh women population) are some other types of crime against women in metro cities of India. Rate of these crimes are significantly lower than other crimes against women. These criminal incidences are localized, have been recorded in very few metro cities. Sixty five Cases of unnatural offences has been recorded in Lucknow, 23 cases in Delhi, 11 cases in Mumbai, 2 cases in Ahmedabad, Hyderabad, Nagpur and Pune, and one case has been recorded in Indore. 85 cases of miscarriage without women consent have been recorded in Lucknow and one such has been recorded in Bengaluru. 18 incidences of acid attack has been recorded in Delhi, 3 cases in Ahmedabad, 2 cases in Kolkata, and one case in Ghaziabad, Indore, Jaipur, Kanpur, Nagpur and Pune. Kolkata (10 cases), Delhi (9 cases), Kochi (6 cases), Bengaluru (4 cases), Nagpur (3 cases), Chennai, Ghaziabad and Hyderabad (1 case) are some of the metro cities in India where some cases of human trafficking has been recorded. Aforementioned four crimes against women are more intense in north Indian metropolitan cities followed by central and south Indian metro cities. The reason behind this spatial variation is more women empowerment in south Indian cities than their northern counterpart, socio-economic differences and higher rate of unemployment in metro cities of north India as compared to south and central Indian metros.

Conclusion : Crime against women is a common phenomena but the intensity of crime against women in metropolitan India is lower than that of overall crime in the study area. The rate of crime against women in metropolitan cities of India is 77.2 crime incidences per one lakh women population. The most common and intense illegal practice against women in metro cities of India is cruelty by husband or his relatives, followed by assault on women with intent to outrage her modesty, kidnapping and abduction, rape or attempt of rape, insult to modesty of women, dowry death, abetment of suicide by women, unnatural offence, causing miscarriage without women consent, human trafficking and acid attack. On average metropolitan cities in northern India have high rate of crime against women followed by metro cities in central India. Metro cities of southern India have lowest crime rate against women. Dowry death, miscarriage without women consent, cruelty by husband or his relatives, kidnapping and abduction and assault on women with intent to outrage her modesty are crimes against women whose intensity is maximum in metro cities of north India. Intensity of crimes like, abetment of suicide of women, acid attack or attempt to acid attack and rape or attempt of rape is highest in metro cities of central India. Human trafficking and insult to modesty of women are more intense criminal activities in metro cities of south India. On the basis of recorded data (in 2016) of crime against women in metropolitan cities of

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Coimbatore in Tamilnadu is safest city for women and Delhi is the most dangerous city for them.

Table-1

Crime against women in metropolitan cities of India: overall statistics (2016)

Name of Metropolitan city	Total number of crime	Number of crime against women	Crime against women (as percentage of total crime)	Crime rate (number of crime per lakh women population)	Rank (on the basis of crime rate)
Ahmedabad	31762	1126	3.55	37.5	13
Bengaluru	49038	3412	6.96	84.0	9
Chennai	113847	544	0.48	12.6	18
Coimbatore	10205	102	1.00	9.5	19
Delhi	206135	13803	6.70	182.1	1
Ghaziabad	12518	1031	8.24	93.7	7
Hyderabad	18295	2419	13.22	64.3	11
Indore	16473	1055	6.40	101.4	6
Jaipur	30477	2090	6.86	144.1	3
Kanpur	9272	1050	11.32	78.4	10
Kochi	54125	392	0.72	36.3	14
Kolkata	24956	1693	6.78	24.9	17
Kozhikode	17491	352	2.01	33.2	15
Lucknow	18869	2205	11.69	159.3	2
Mumbai	59072	5128	8.68	60.2	12
Nagpur	42866	1379	3.22	113.0	5
Patna	16769	1284	7.66	133.8	4
Pune	19554	2131	10.90	89.2	8
Surat	56943	565	1.00	28.7	16
Total	808637	41761	5.16	77.2	

Source: National Crime Record Bureau report, 2016.

Table-2

Crimes against women in metropolitan cities of India (2016)

Name of metropolitan city	Dowry death		Abetment Of suicide of women		Causing miscarriage without women's consent		Acid attack or attempt of acid attack		Cruelty by husband or his relatives		Kidnapping Or abduction of women	
	I	R	I	R	I	R	I	R	I	R	I	R
Ahmedabad	02	0.1	21	0.7	00	0.0	03	0.1	562	18.7	271	9.8
Bengaluru	57	1.4	76	1.9	01	0.0	00	0.0	489	12.0	674	16.9
Chennai	05	0.1	37	0.9	00	0.0	00	0.0	178	4.1	15	0.3
Coimbatore	01	0.1	00	0.0	00	0.0	00	0.0	37	3.5	04	0.4
Delhi	144	1.9	20	0.3	00	0.0	18	0.2	3645	48.1	3364	44.4
Ghaziabad	20	1.8	00	0.0	00	0.0	01	0.1	481	43.7	215	21.4
Hyderabad	18	0.5	30	0.8	00	0.0	00	0.0	1311	34.0	227	6.0
Indore	19	1.8	25	2.4	00	0.0	01	0.1	275	26.4	230	22.1
Jaipur	31	2.1	09	0.6	00	0.0	01	0.1	1008	69.8	177	26.0
Kanpur	50	3.7	12	0.9	00	0.0	01	0.1	365	27.2	118	21.1
Kochi	01	0.1	00	0.0	00	0.0	00	0.0	111	10.3	25	2.3
Kolkata	10	0.1	21	0.3	00	0.0	02	0.1	886	13.0	129	1.8
Kozhikode	02	0.2	00	0.0	00	0.0	00	0.0	161	15.2	06	0.6
Lucknow	42	3.0	09	0.9	85	6.2	00	0.0	895	61.9	601	43.6
Mumbai	12	0.1	27	0.3	00	0.0	00	0.0	582	6.9	1142	13.4
Nagpur	06	0.5	12	2.6	00	0.0	01	0.1	248	20.1	368	30.2
Patna	76	7.9	00	0.0	00	0.0	00	0.0	105	12.2	362	38.5
Pune	10	0.4	18	1.6	00	0.0	01	0.1	329	18.9	578	24.5
Surat	00	0.0	12	0.6	00	0.0	00	0.0	195	9.9	162	8.2
Total	506	6.9	360	0.7	86	0.2	29	0.1	12218	22.6	9256	17.1

Source: National Crime Record Bureau report (2016); I- Number of incidence, R- rate of crime (per lakh women).

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Table- 2 : Crimes against women in metropolitan cities of India (2016)

Name of metropolitan city	Human Trafficking		Rape or attempt of rape		Unintentional offences		Assault on women with intent to outrage her modesty		Insult to modesty of women	
	I	R	I	R	I	R	I	R	I	R
Ahmedabad	00	0.0	112	3.7	02	0.1	131	4.3	62	0.3
Bengaluru	04	0.1	324	8.0	00	0.0	270	20.2	51	1.3
Chennai	01	0.0	25	0.6	00	0.0	63	1.5	63	0.1
Cochin	00	0.0	00	0.0	00	0.0	19	1.3	00	0.0
Delli	09	0.1	2025	26.7	23	0.3	1746	49.3	743	10.3
Ghaziabad	01	0.1	117	10.6	00	0.0	172	15.6	295	3.3
Hyderabad	01	0.0	170	4.5	02	0.1	222	21.3	92	3.3
Indore	00	0.0	181	17.4	01	0.1	301	20.8	69	0.0
Jaipur	00	0.0	334	23.1	00	0.0	154	11.5	01	0.1
Kanpur	00	0.0	55	4.1	00	0.0	162	15.0	23	2.1
Kochi	06	0.6	62	5.8	00	0.0	348	5.1	243	3.6
Kolkata	10	0.1	18	0.2	00	0.0	109	10.3	19	1.3
Kozhikode	00	0.0	52	4.9	00	0.0	412	29.9	00	0.0
Lucknow	00	0.0	102	7.4	65	4.7	2183	25.6	425	5.0
Mumbai	00	0.0	713	3.4	11	0.1	411	33.7	04	0.3
Nagpur	03	0.2	171	14.0	02	0.2	102	10.6	03	0.3
Patna	00	0.0	63	6.5	00	0.0	661	27.7	56	2.3
Pune	00	0.0	354	14.8	02	0.1	55	2.8	00	0.0
Surat	00	0.0	121	6.1	00	0.0	10458	19.3	1917	3.5
Total	35	0.1	4999	9.2	108	0.2				

Source: National Crime Record Bureau report (2016); I- Number of incidence, R- rate of crime (per lakh women).

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Biological, Electronic, NLO, NBO, TDDFT and Vibrational Analysis of 1-benzyl-4-formyl-1H-pyrrole-3-carboxamide

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ABSTRACT: *Biological Electronic, Optical Properties and Vibrational Analysis of 1-benzyl-4-formyl-1H-pyrrole 3carboxamide are studied by using a combination of DFT/B3LYP method and 6-311G (d, p) basis set. Optimized parameters of the title molecule are well-matched with the experiments. The NLO properties of 1-benzyl-4-formyl-1H-pyrrole 3carboxamide have been examined with the help of Polarizability and Hyper-Polarizability. The electronic properties of 1-benzyl-4-formyl-1H-pyrrole 3carboxamide are described with the help of HOMO, LUMO composition. The UV spectra suggest that a strong excitation line occurs at 2.03 eV (160 nm) due to H-2→LUMO (30%). NBO analysis shows that hyper conjugative interaction energy has higher value during LP→π*, π→π* transitions. Several biological activities are calculated by PASS software. Docking of the molecule is performed with 5P4Q protein and FF score is -1051.65A.U.*

KEYWORDS: *Vibrational analysis; NBO; NLO; DFT; Electronic properties; PASS.*

INTRODUCTION

Quantum Chemical calculations give important information about molecular geometry, vibrational frequency, electronic properties, UV spectra analysis as well as NLO properties of a molecule. [1-2] Benzyl is the substituent possessing the benzene ring attached to a CH₂ group (C₆H₅CH₂-). [3] The position of the first carbon bonded to benzene or another aromatic ring is described as benzyl. The 4-formyl-1H-pyrrole-3 carboxamide is a heterocyclic aromatic organic compound

in which three hydrogen of Pyrrole ring (five-membered) replaced by formyl, carboxamide, and Benzyl group. Heterocyclic compounds are those cyclic compounds that contain at least two different elements as 'ring members' atoms. These compounds are organic or inorganic, within the ring structure containing one carbon atom, and one or more atoms of elements other than carbon, such as sulphur, oxygen, nitrogen, etc. Simple N heterocycles have acknowledged significant consideration because of

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their important biological properties and their role as pharmacophores. [4.] The introduction of acyl group on nitrogen atom of pyrrole possesses medicinal importance. [5]. In chemistry, formylation is termed as addition of formyl functional group. Formylation has been identified in several critical biological processes [6]. Pyrrole rings have pharmacological as well as biological implications [7]. The derivatives of Pyrroles are very important in drug discovery. [8] These derivatives are used as pharmacological activity such as anti-inflammatory [9], antibacterial [10-13], antioxidant [14] and antitumour agents [15]. Qi-Di Zhong et al. synthesized new pyrrole derivatives 1-benzyl-4-formyl-1H-pyrrole 3carboxamide with good biological activities, and also reported its crystal structure. The present work on 1-benzyl-4-formyl-1H-pyrrole 3carboxamide has been carried out to support and as an extension of the work of Qi-Di Zhong et al. [16] In this paper we perform a complete quantum chemical study of 1-benzyl-4-formyl-1H-pyrrole 3carboxamide by using combination DFT/B3LYP method and 6-311G (d, p) basis set. To verify its biological activity several biological activities have been calculated using PASS software and docking is performed by appropriate target.

Computational Methods

Initial geometry of the molecule is modeled with the help of Gauss View 5.0 by using standard parameters. Geometry optimization is done without any constraint in the potential energy surface. The gradient corrected Density Functional Theory (DFT) with the three-parameter hybrid functional (B3) [17] for the exchange part and the Lee-Yang-Parr (LYP) correlation function [18] has been employed for the computation of molecular structure, vibrational frequencies, HOMO-LUMO, by using GAUSSIAN 09 [19]. Vibrational frequency assignments were made with a high degree of accuracy by combining the results of the GAUSSVIEW'S program [20] with symmetry considerations. In this study, 6-311G(d, p) basis set with d polarization function for heavy atoms and p polarization function for hydrogen atom is used. 6-311G(d, p) basis set gives better description of polar bond in our study. [21-22] Natural bond analysis is calculated by NBO3.0 program package [23].

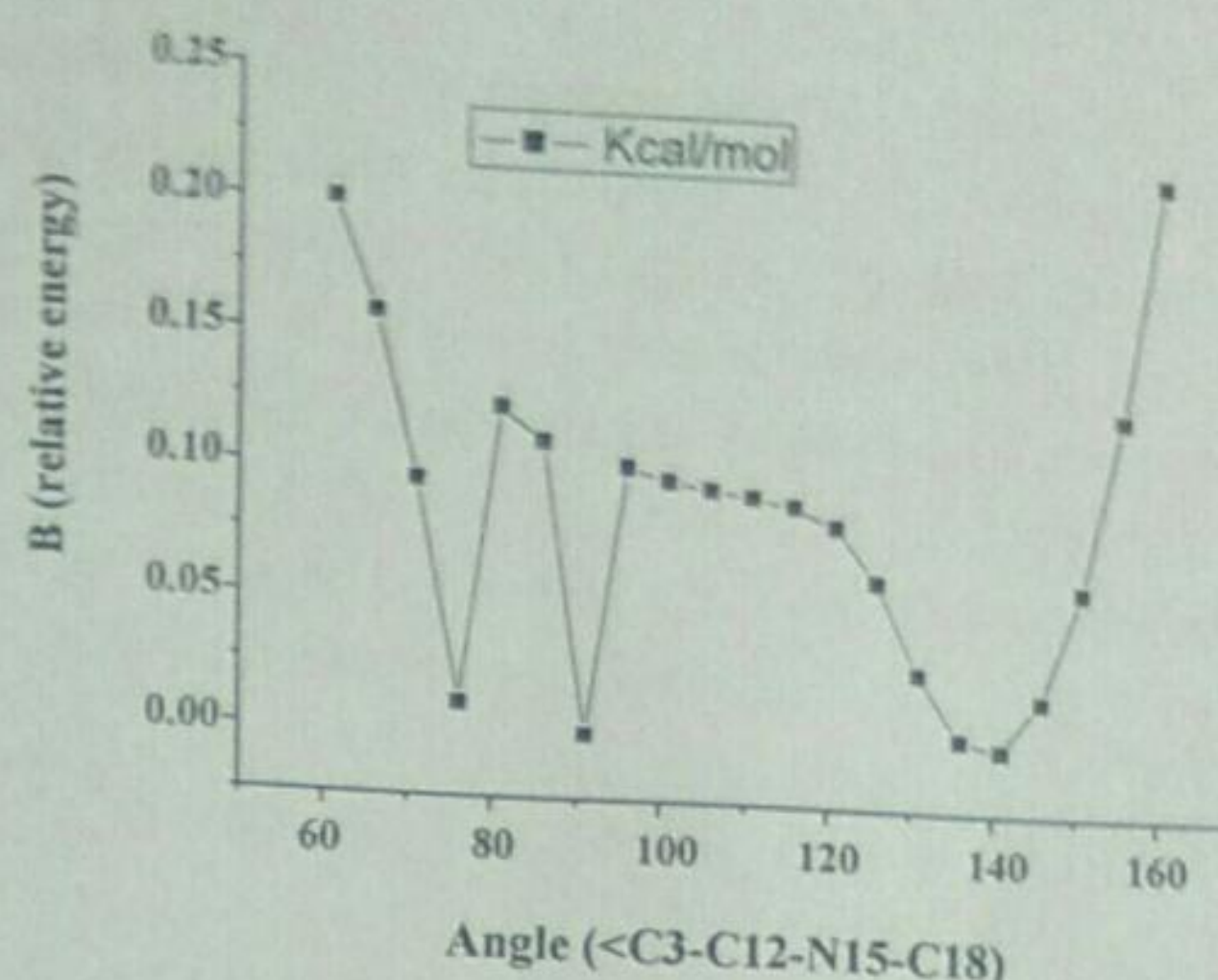


Fig. 1: PES Scan of dihedral angle $\angle 3C-12C-15N-18C$ with 20 step each of 5° .

RESULTS AND DISCUSSIONS

Optimization

The local minimum energy obtained by structure optimization of the molecule is approximately 716.02957909 A.U. Animated gauss view picture shows that the molecule has no point group symmetry. For optimized parameters bond length is measured in Å and bond angle in degrees. To obtain global minima we scan dihedral angle $\angle 3C-12C-15N-18C$ with 20 step each of 5° and then plot a graph (Fig. 1) in between relative energy and dihedral angle. From this plot, conformer with dihedral angle $\angle 3C-12C-15N-18C = 91.147^\circ$ (shown Fig. 3) has the lowest energy. This conformer has 0.01041 kcal/mol lower energy than next stable conformer with $\angle 3C-12C-15N-18C = 76.147^\circ$. For sake of simplicity we have considered the most stable conformer for our study. In the molecule there are two rings namely pyrrole and benzyl rings, nearly perpendicular, are connected with methyl group. The calculated geometry parameter are compare with experimental data in Supplementary Table 1. The calculated (C-N) bond length, lies in between 1.3976Å- 1.3488Å, is in agreement with experimental results [16](1.37Å -1.36Å) while calculated (N-H) bond length lies in between 0.9973Å- 0.9937Å, which matches with experimental value (1 Å). The C-O bond length is found to be 1.37 Å however experimental value is 1.29 Å. In Fig. 2 we plot a graph between experimental and calculated bond length of the molecule. Graph shows linear relation and after linear correlation between experimental bond lengths with calculated bond length by DFT method we find correlation equation

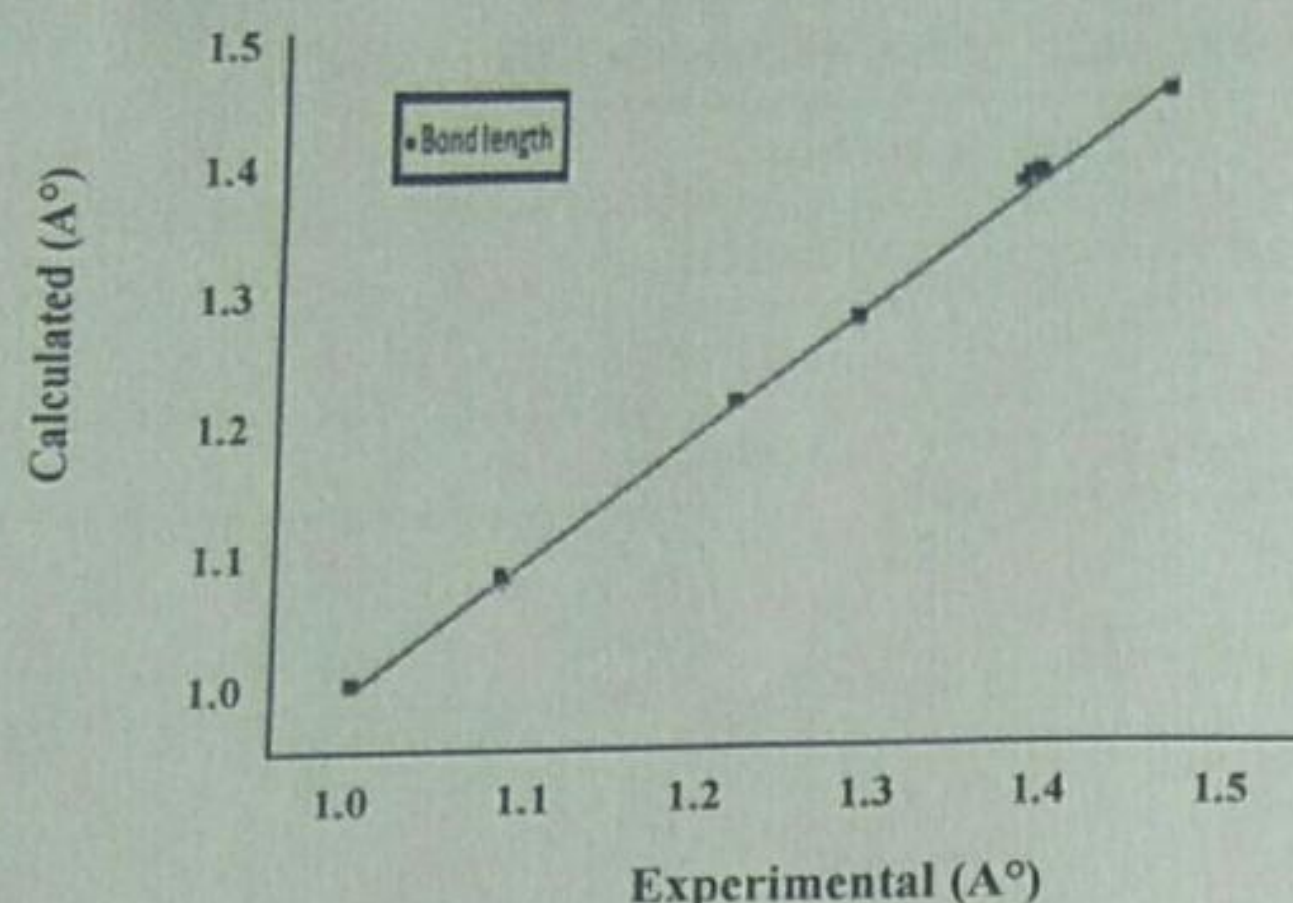


Fig. 2: Comparison between experimental and theoretical bond length.

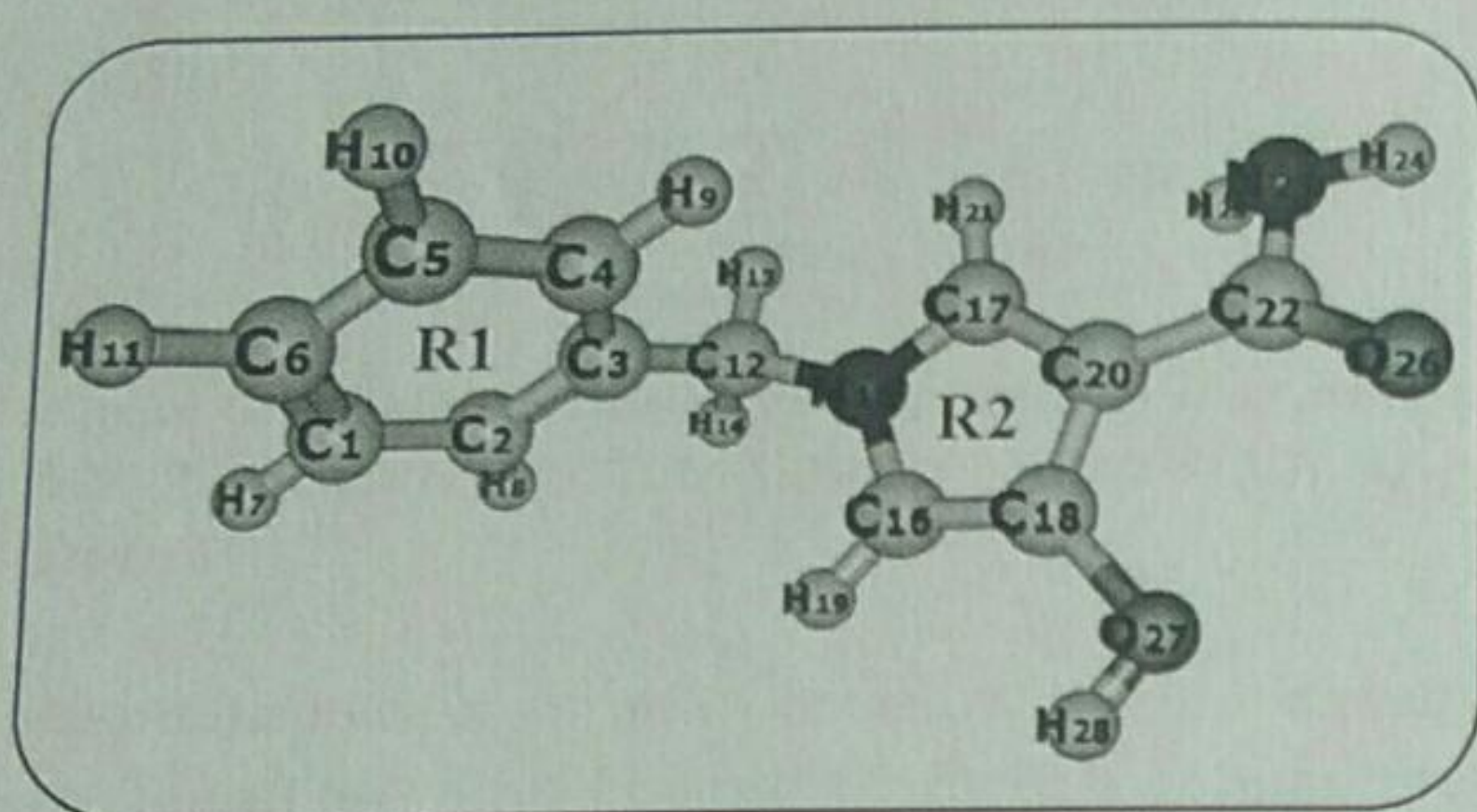


Fig. 3: Model molecular structure of 1-benzyl-4-formyl-1H-pyrrole-3-carboxamide.

Calculated = 0.98062 experimental + 0.01911
with correlation factor $R^2=0.99861$.

The correlation factor >0.99 shows that the DFT can reproduce experimental result well. The angular changes in benzene ring geometry have proved to be a sensitive indicator of the interaction between the substituent and the attached ring. The (C-N-C) bond angle varies from 124.82° - 109.40° while (C-N-H) varies between 181.07° - 123.24° .

Polarizability, Hyper polarizability and thermodynamic properties

The Dipole moment (μ), polarizability $\langle\alpha\rangle$ and total first static hyper polarizability β are used to determine NLO property of title molecule.[24-25] These parameter are calculated by using combination of DFT/B3LYP method and 6-311G(d, p) basis set (supplementary Table-2). First order hyperpolarizability is a third rank tensor of $3\times3\times3$ matrix. By using Kleinman symmetry,

consideration 27 components of the 3-D matrix can be reduced to 10 components.[26] Polarizability and hyperpolarizability belongs to first and higher order derivatives of the electron density which is helpful to determine shape and interaction characteristics of chemical bond in molecule. These parameter can be expressed in terms of x, y, z components and are given by following equations 1, 2, 3

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

$$\langle\alpha\rangle = 1/3[\alpha_{xx} + \alpha_{yy} + \alpha_{zz}] \quad (2)$$

$$\beta_{\text{Total}} = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1/2} = [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yxx} + \beta_{yzz})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2]^{1/2} \quad (3)$$

The β components of Gaussian output are reported in atomic units.

Where (1 a.u. = 8.3693×10^{-33} e.s.u.).

For 1-benzyl-4-formyl-1H-pyrrole-3-carboxamide molecule, calculated dipole moment value is 4.2863 Debye which is greater than dipole moment of water (2.16 Debye), is attributed to electron withdrawing group $-\text{COONH}_2$ - and $-\text{OH}$ - group present on hetro-cyclic ring. From supplementary Table 2 we see higher contribution of axial component in polarizability shows that molecule is elongated more towards axial direction. In hyperpolarizability β_{xxx} , β_{zzz} component having larger contribution shows that a larger electron density along bond along X direction and XZ plane. This shows that X axis and XZ plane are more optical active directions. The calculated values for the total intrinsic hyperpolarizability β_{TOTAL} and the component of the hyperpolarizability ($\bar{\beta}$) are given in supplementary Table 2. The calculated value β_{TOTAL} of title molecule (0.9339×10^{-30} e.s.u.) is nearly five times greater than hyperpolarizability of urea (0.19347×10^{-30} e.s.u.) so title molecule use as NLO active molecule

Thermodynamical Properties

Thermodynamic properties like entropy, enthalpy and heat capacity at various temperatures (100-400 K) have been calculated (Fig. 4) by DFT/6-311G(d, p) method from the theoretical vibration analysis. These parameters increase with temperature. The graphs between

Table 1: The observed UV-vis spectra are calculated by TD-DFT method at B3LYP/6-311 G (d, p) level.

Excitation energy (eV)	wavelength (nm)		Oscillator strength	Orbital transition
	Calculated	Assignment		
4.12	250.62	$n \rightarrow \pi^*$	0.0008	H-4→L+1 (26%)
2.03	160.20	$\pi \rightarrow \pi^*$	0.2305	H-2→LUMO (30%)

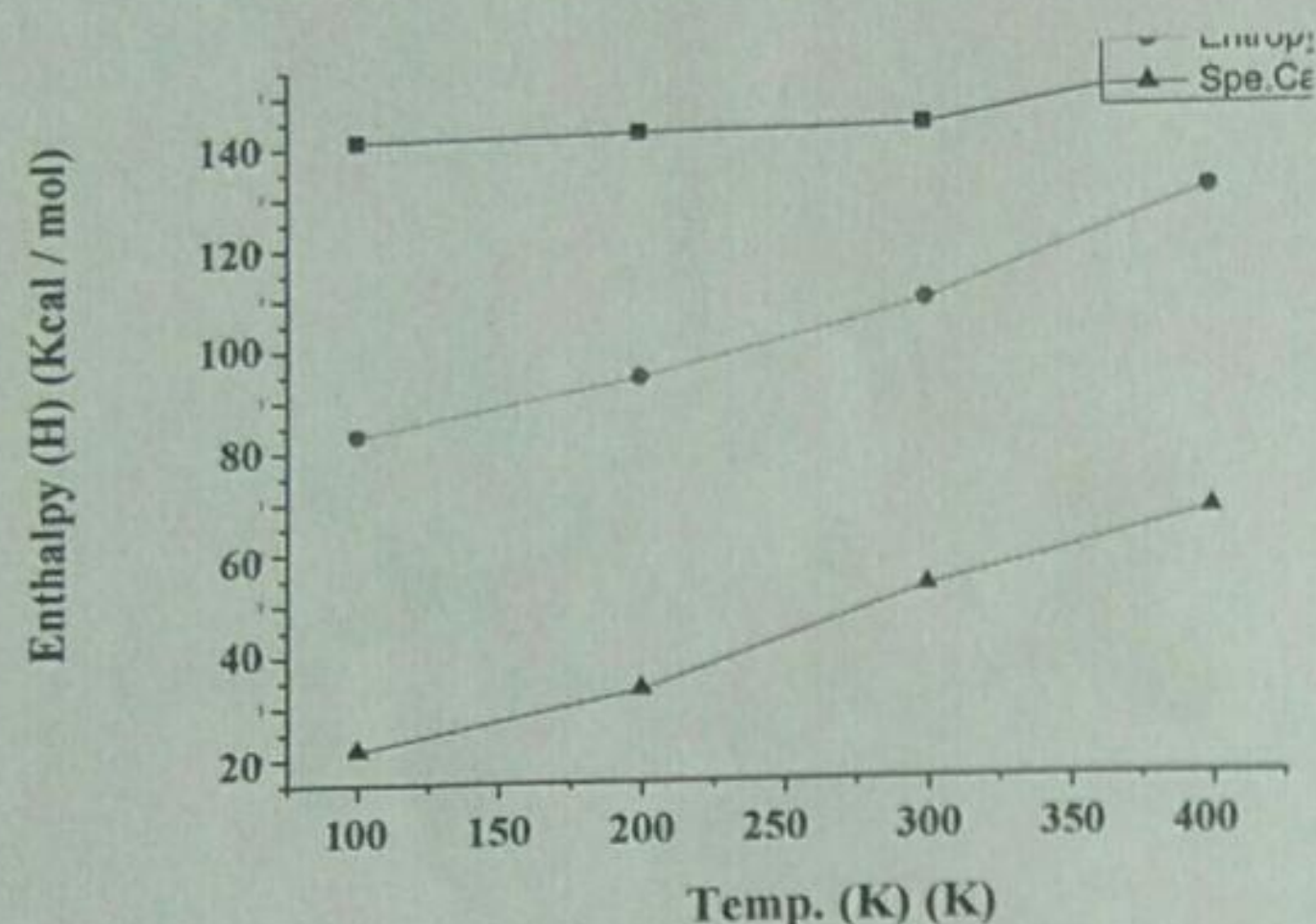


Fig. 4: Graph plotted between entropy enthalpy Heat capacity V/S Temperature (K) calculated by DFT/6-311G (d, p) method.

temperature-entropy and enthalpy -heat capacity are plotted and fitted in quadratic formula of order two. The fitting factors for these calculated thermodynamic properties are 0.97519 (for C), 0.99873 (S) and 0.9899 (H), respectively, while the second order quadratic fitting equations are as follows

$$H_m^0 = 147.1585 - 0.07799T + 0.000221T^2 \quad (R^2 = 0.9899)$$

$$C_{p,m}^0 = 8.503 + 0.11861T + 0.000067T^2 \quad (R^2 = 0.97519)$$

$$S_m^0 = 78.14075 + 0.02638T + 0.000247T^2 \quad (R^2 = 0.99873)$$

These quadratic equations give significant information about thermochemical field to calculate thermodynamic energy.

Electronic Properties and UV Spectra

The interaction of the molecule with other chemical system is resolute by frontier orbitals, FHOMO and FLUMO which can be verified by experimental data. The frontier orbital gap is equal to HOMO-LUMO gap which helps to determine the kinetic stability and chemical reactivity of the molecule. The molecule is termed as soft molecule when it becomes more polarizable, high chemically reactive, low kinetically stable and have small frontier orbital gap. [27] The frontier orbital gap calculated for given molecule is 6.20 eV, shows molecule

is less chemically active. The contour plots of HOMO, LUMO orbital and MESP of the molecule are shown in Fig. 4. In this plot HOMO, which primarily acts as donor is distributed over R₂ ring of the molecule while LUMO behaves as acceptor distributed over benzene ring. The transition from HOMO→LUMO shows that charge is transferred from ring R₂ to benzene ring.

The MESP plot gives valuable information about reactive site to positive, negative, and neutral electrostatic potential region in terms of color coding e.g red as electro negative, blue as electro positive and yellow as neutral site[28-30]. MESP of the molecule visibly suggests that the major electronegative potential region (shaded with Red colour) O₂₇, O₂₆ atoms of -CONH₂- group and most electropositive region C₂₂ (shaded with blue colour).

UV spectra TDDFT analysis

Time dependent density theory is important tool for the study of the nature of transition of electron in title compound. After optimization by using combination of DFT/B3LYP method and 6-311G (d, p) basis set, we have used TD-DFT calculation with same level theory to find energy of various transition state. The calculated electronic transition energies (Table 1) at 4.12 eV (250.62 nm) and 2.03 eV (160.20 nm) mainly originate due to H-4→L+1(26%), H-2→LUMO(30%) transitions respectively. The plot and transition of HOMO-4(MO=53), H-2(MO=55), LUMO (MO=58) LUMO+1(MO=59) of the molecule is shown in Fig. 6. HOMO-2 is localized over Benzene ring (as HOMO) however HOMO-4 is localized over -CONH₂-group. The LUMO and LUMO+1 are nearly localized over whole molecule. So the transitions from H-4→L+1 and H-2→LUMO show that charge transfer from benzene and -CONH₂- group to R₂ ring. A graph is plotted between wavenumber and oscillatory strength and shown in Fig. 5. On the basis of the calculated molecular orbital coefficients analyses electronic transition are assigned to $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ respectively.

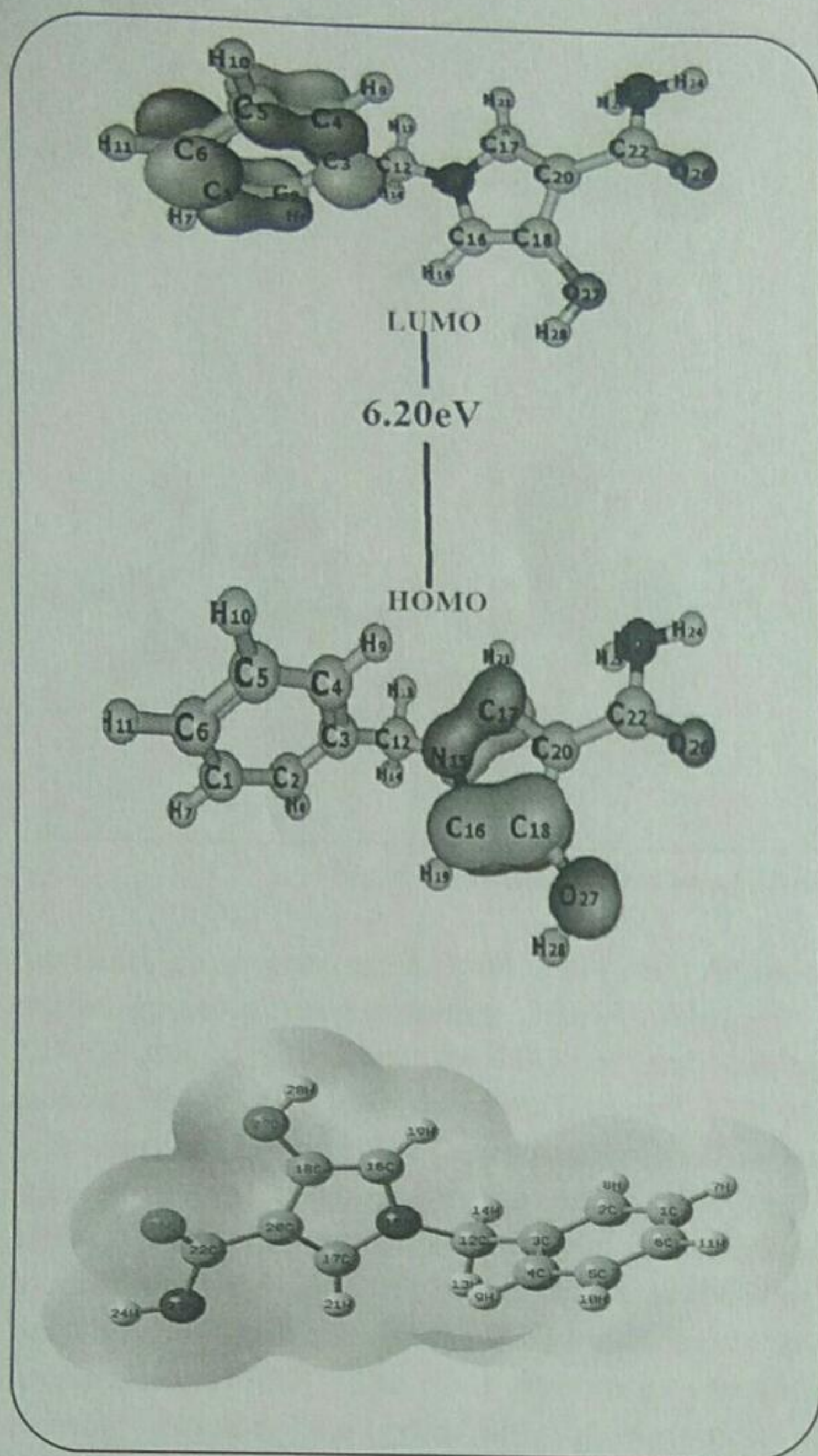


Fig. 4: HOMO - LUMO MESP pictures of 1-benzyl-4-formyl-1H-pyrrole-3-carboxamide

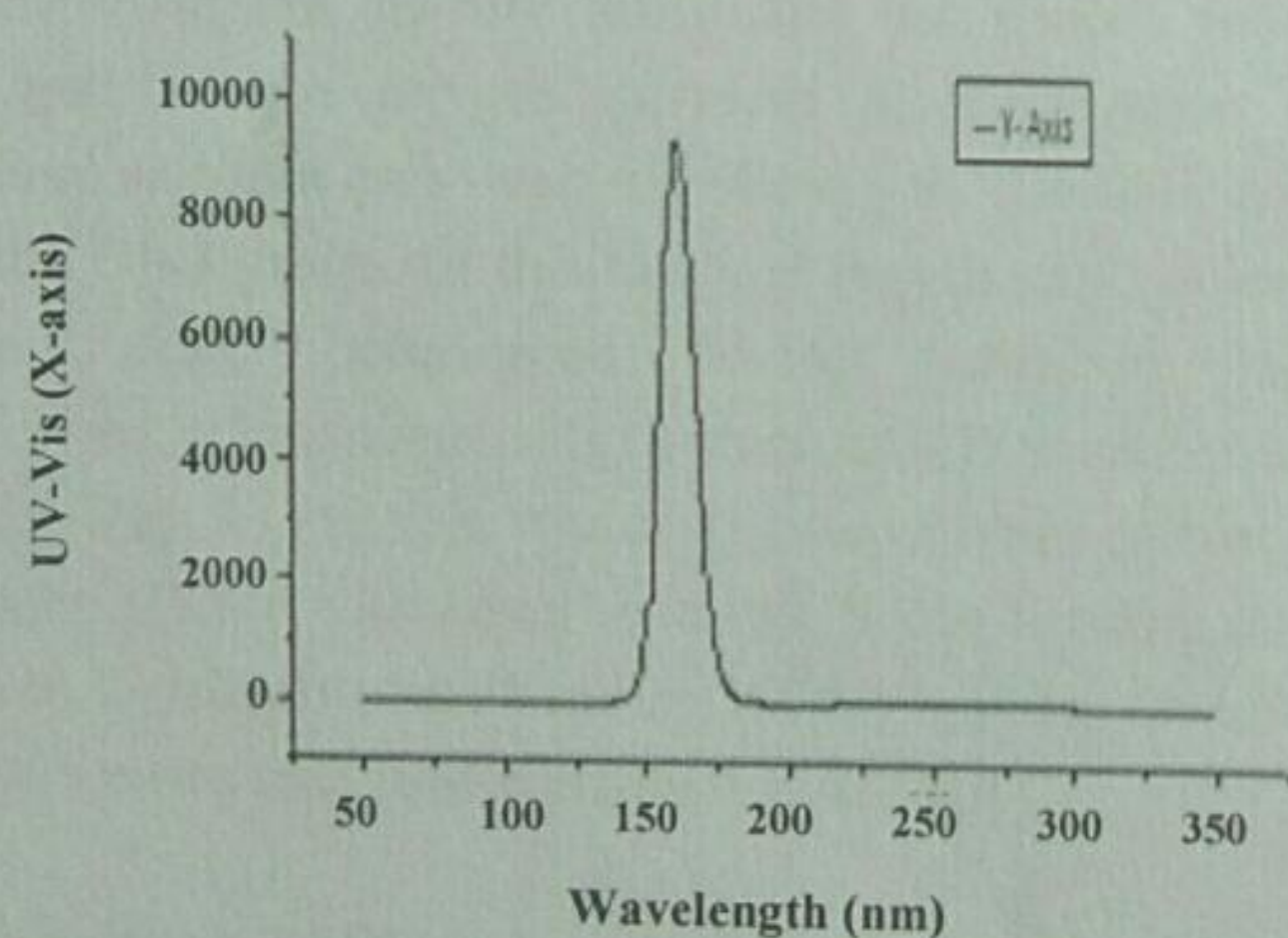


Fig. 5: Calculated UV spectra of Title molecule using combination of DFT/B3LYP method and 6-311G(d,p) basis set.

Assignments of Fundamentals

In 1-benzyl-4-formyl-1H-pyrrole-3-carboxamide has 28 atoms 78 normal modes of vibration. The assignments of the calculated wave numbers are based on animated view of normal mode and listed in supplementary Table 3. The calculated frequencies are typically higher than the experimental one due to combination of electron correlation and anharmonicity. [31-32] Due to this reason the theoretical frequency is scaled. Vibrational frequencies are scaled by the factor of 0.96 [33]. Some important modes of vibrations are discussed here.

Vibrational modes description

Ring vibration

The presence of C-H stretching vibrations in the region $2800-3100\text{ cm}^{-1}$, which is the characteristic region for identification of the C-H group.[33] In the molecule the C-H functional group is present at a number of positions. Three medium intense polarized peaks with polarization vectors directed along ring R₁ appear at 3231 cm^{-1} , 3240 cm^{-1} and 3251 cm^{-1} due to $\nu(\text{C-H})$ R₁. Two medium intense polarized peaks lying on lower side of spectral region due to $\beta(\text{C-H})$ R₁ and $\gamma(\text{C-H})$ R₁ are at 1562 cm^{-1} , 778 cm^{-1} respectively. An intense and a medium intense peaks occur due to mixing of $\nu(\text{C=C})$ R₁, $\beta(\text{C-H})$ R₁ corresponding to 1743 cm^{-1} and 1562 cm^{-1} respectively. A very intense peak occurs due to mixing of in plane $\text{O}_{27}\text{-H}_{28}$ bending $\text{C}_{16}\text{-N}_{15}$ stretching in ring R₂ is at 1470 cm^{-1} . The $\mu(\text{C}_{16}\text{-N}_{15})$ appears as a prominent mode in the FT-IR spectra at 1686 cm^{-1} . Three back to back sharp peak appears due to stretching of $\text{C}_{16}\text{-N}_{15}$ bond in ring R₂ appears at 1472 cm^{-1} , 1500 cm^{-1} , 1529 cm^{-1} . A very weak intense peak appears at 1115 cm^{-1} due to in plane bending $\text{C}_{16}\text{-N}_{15}\text{-C}_{17}$ in ring R₂ however at lower range of spectra two intense peak appears due to $\gamma(\text{C}_{16}\text{-N}_{15}\text{-C}_{17})$ R₂ appears at 928 cm^{-1} and 684 cm^{-1} respectively.

-CONH₂-group vibration

The -NH_2 and -C=O functional groups are noteworthy elements of the molecule and vibrations corresponding to these groups are present in a number of modes. The N-H stretching vibration generally obtained in the region of $3500\text{-}3000\text{ cm}^{-1}$ [34]. In this study at higher frequency region two intense modes due to antisymmetric and symmetric stretching of NH_2 in -CONH_2

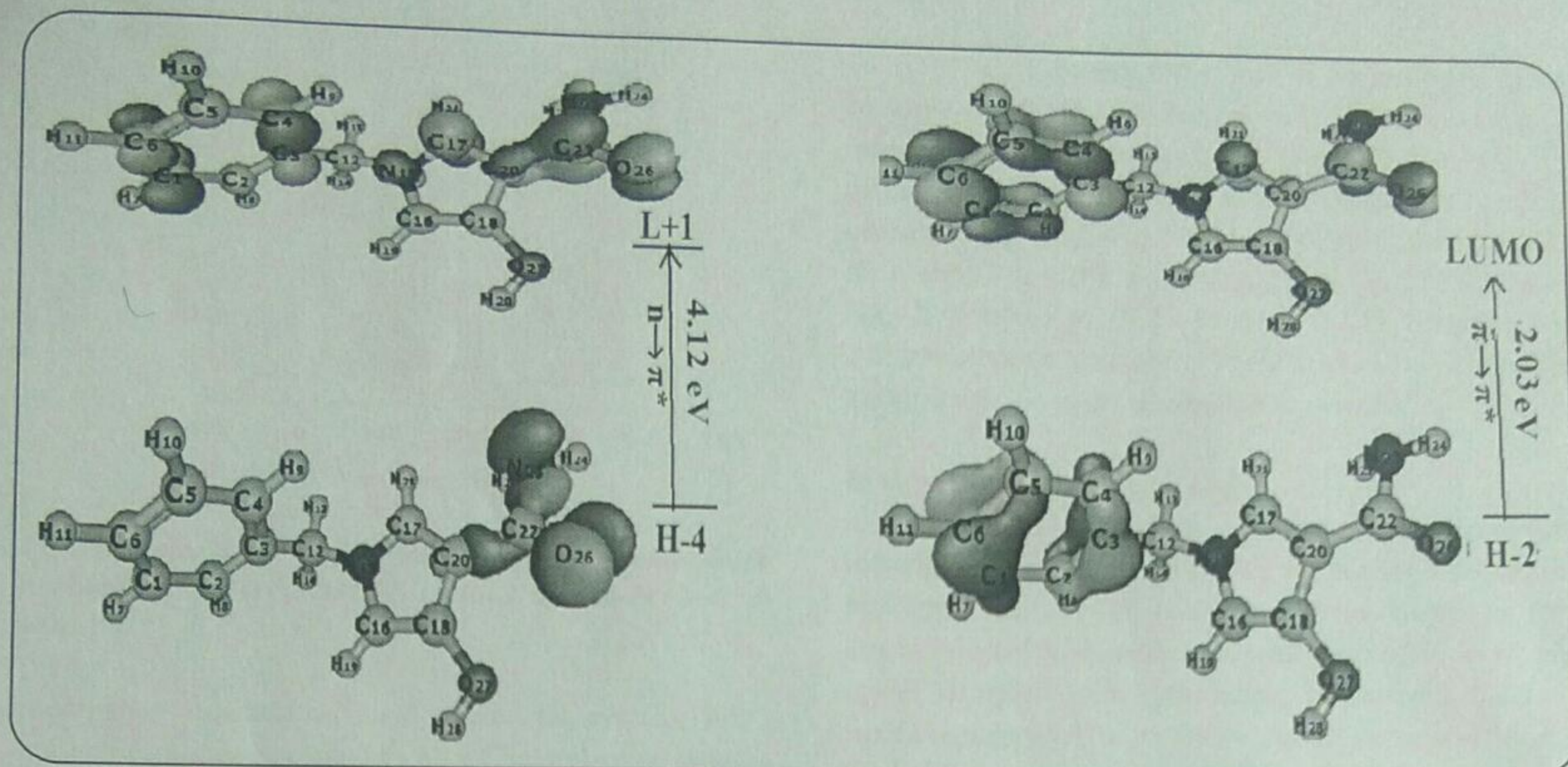


Fig. 6: Electronic Transition of TD-DFT of title molecule by DFT/B3LYP method.

functional group occur at 3637 cm^{-1} , 3554 cm^{-1} . At lower region frequency two scissoring $S(\text{H}_{24}\text{-N}_{23}\text{-H}_{25})$ of $-\text{CONH}_2$ group are 1682 cm^{-1} and 1145 cm^{-1} and wagging modes $\omega(\text{H}_{24}\text{-N}_{23}\text{-H}_{25})$ R_2 obtained are 1184 cm^{-1} , 1226 cm^{-1} , 856 cm^{-1} and 611 cm^{-1} . The $\text{C}=\text{O}$ stretching band having high intensity is obtained in the region 1800 cm^{-1} - 1650 cm^{-1} [35.], however their exact position is governed by the inter and intra molecular hydrogen bonding, electronic and mass effects of adjacent substituents and conjugations [36-37]. The $\text{C}-\text{O}$ stretching vibrations intensity increases the probability of formation of hydrogen bonds. The $\text{C}=\text{O}$ bond is produced by $p_\pi - p_\pi$ between carbon and oxygen atoms. In $\text{C}=\text{O}$ bond bonding electron are not equally distributed but shifted towards oxygen because oxygen is more electronegative than carbon and lone pair electron of oxygen decides nature of the $\text{C}=\text{O}$ group. In this study a very intense polarized band with polarization vector directed along the plane of adjacent ring occurs at 1785 cm^{-1} due to $\mu(\text{C}_{22}\text{-O}_{26})$ R_2 . In this stretching mode both carbon and oxygen vibrate with equal intensity. Some bending modes due to $\text{C}_{22}\text{-O}_{26}$ in plane bending modes appears lower side of IR spectra with low intensity e.g. 627 cm^{-1} .

Other Modes of Vibration

Pulay *et al* [38] recommended the vibrational frequencies on the basis of internal coordinate system.

NH_2 and CH_2 group connect with six types of vibrational frequencies namely: two stretching modes symmetric, asymmetric and rest four bending modes e.g., scissoring, rocking, wagging and twisting. In which two scissoring and rocking deformations belong to polarized in-plane vibration however wagging as well as twisting deformations belong to depolarized out-of-plane vibration.

In calculated spectra one low intense polarized peak with polarization vector is directed along $\text{C}_{17}\text{-N}_{15}$ at 3140 cm^{-1} due to $\mu_{as}(\text{H}_{14}\text{-C}_{12}\text{-H}_{13})$ adj R_1 and a medium intense peak occurs at 3097 cm^{-1} due to symmetric $\mu_s(\text{H}_{14}\text{-C}_{12}\text{-H}_{13})$ stretching vibration. On the lower side of spectra, two intense peaks due to scissoring modes of vibration, occur at 1612 cm^{-1} and 1460 cm^{-1} . A very intense polarized peak occurs at 1472 cm^{-1} with polarization vector directed along bond $\text{C}_{17}\text{-H}_{21}$ due to $S(\text{H}_{14}\text{-C}_{12}\text{-H}_{13})$ adj R_2 . At higher frequency region an intense polarized peak at 3760 cm^{-1} with polarization vector directed along $\text{N}_{15}\text{-C}_{16}$ due to $\mu(\text{O}_{27}\text{-H}_{28})$ R_2 occurs. From lower side of IR spectra two intense peaks occur at 709 cm^{-1} , 713 cm^{-1} due to $\gamma(\text{O}_{27}\text{-H}_{28})$ R_2 . The $\text{O}-\text{H}$ group present in our molecule is expected to be most sensitive which shows noticeable shifts in the spectra of the hydrogen-bonded species.

NBO analysis

Natural bond orbital analysis is used to study interaction among the bond and charge transfer or

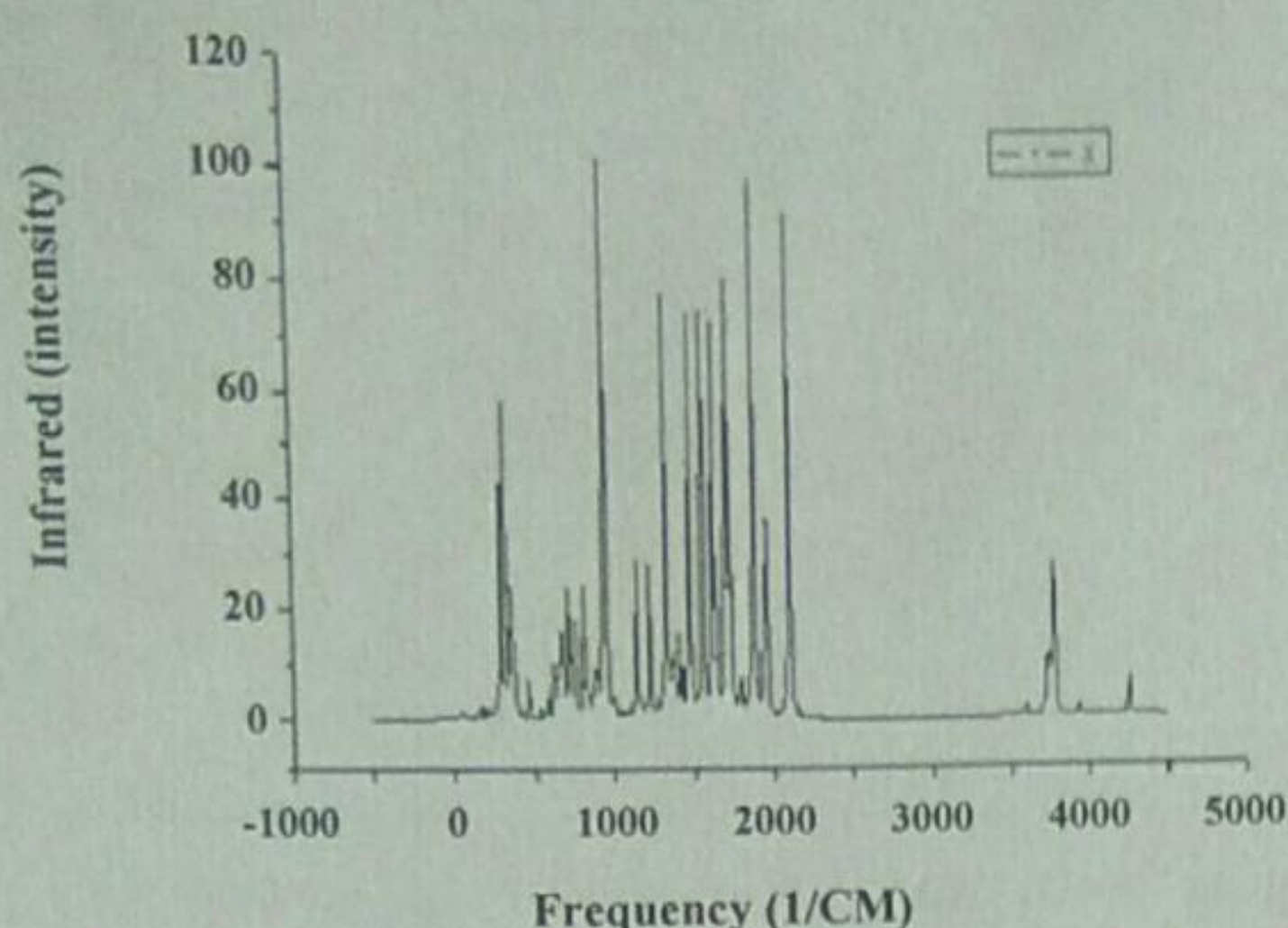


Fig. 7: Calculated IR spectra of Title molecule using combination of DFT/B3LYP method and 6-311G(d, p) basis set.

conjugative interactions in a molecular system. NBO analysis provides information about how electron density gets transferred from the bonding orbitals to the antibonding orbitals [39]. The strength of these interactions depends on the value of the second order energy of interaction between the donor and acceptor orbitals. The interaction between electron donors and electron acceptors is intense if the value of $E^{(2)}$ is high. The second order energy lowering is calculated by using each donor $NBO(i)$ and acceptor $NBO(j)$ and the strength of delocalization interaction [40]

$$E^{(2)} = -q_i \frac{F_{ij}}{\epsilon_j - \epsilon_i}$$

Several significant interactions are listed for the study molecule in Supplementary Table 4. From this table it is clear that σ electron density (1.976e - 1.983e) shows higher value than π electron density (1.862e - 1.665e). In this molecule mainly $\sigma \rightarrow \sigma^*$, $\pi \rightarrow \sigma^*$, $\pi \rightarrow \pi^*$, $LP \rightarrow \pi^*$, σ^* interactions occur between bonding and antibonding orbitals i.e. The $\sigma \rightarrow \sigma^*$ interactions between bonding and antibonding orbitals are found to be σ (C23-C25) $\rightarrow \sigma^*$ (C22-O26) and σ (C16-C18) $\rightarrow \sigma^*$ (C18-C21), having $E^{(2)}$ values of 10.04 kcal/mol and 4.15 kcal/mol respectively. The $\pi \rightarrow \sigma^*$ interactions between bonding and antibonding orbitals which stabilized molecule is found to be π (C2-C3) $\rightarrow \sigma^*$ (C4-C5) with $E^{(2)}$ 45.21 kcal/mol. The $\pi \rightarrow \pi^*$ interactions between bonding and antibonding orbitals are π (C1-C6) $\rightarrow \pi^*$ (C2-C3), π (C1-C6) $\rightarrow \pi^*$ (C4-C5), π (C4-C5) $\rightarrow \pi^*$ (C2-C3), π (C4-C5)

$\rightarrow \pi^*$ (C1-C6), having $E^{(2)}$ values 46.69 kcal/mol, 46.75 kcal/mol, 48.01 kcal/mol and 45.21 kcal/mol respectively. The strongest interaction $LP \rightarrow \pi^*$ / σ^* involving lone pairs and nearly vacant antibonding orbitals such as $LP(1) N15 \rightarrow \pi^*$ (C16-C18) and $LP(1) N22 \rightarrow \pi^*$ (C17-C20) and $LP(2) O26 \rightarrow \sigma^*$ (C22-N23) have high $E^{(2)}$ values of 67.11 kcal/mol 72.42 kcal/mol and 24.69 kcal/mol respectively. These interactions contribute the greatest role to stabilizing the molecule.

Biological activity and docking

PASS [41] predicts Methylene tetrahydrofolate reductase to be inhibitor (0.7610) and having Antiallergic biological activity (0.7180), which is based on the structure activity relationships with $Pa > 0.70$. In methyl cycle Methylene tetrahydrofolate, reductase is the rate-limiting enzyme. The molecule under study inhibits this enzyme and prevents the human body from Alzheimer, other forms of dementia, colon cancer and acute leukemia disease. The molecule shows better activity against allergic diseases which are caused by hypersensitivity of the immune system typically harmless substances in the environment [42]. Swiss dock [43] is an online webserver, which predicts suitable binding protein for the molecule is 5P4Q [44]. The structure 5P4Q has in total one chain with sequence from *Cryptosporidia* parasite. The *Cryptosporidia parasitica* is a fungus belonging to Ascomycota taxon pathogen. It is the main cause of chestnut disease, a shocking disease of the American chestnut trees. [45]

After predicting suitable protein we perform docking of the molecule with the trial protein 5P4Q by Swiss Dock web server. All the probable conformers of the ligand and their corresponding energy values are resolved and best binding modes are ranked according to the full fitness (FF). This docking process is not covered on specific region of the chosen protein but blind follows whole region of chosen protein. The highest negative values of full fitness score show the best binding site between protein and the taken molecule. The full fitness score obtained in docking is -1051.65 A.U. Docking between title molecule and 5P4Q protein is shown in Fig. 8 using UCSF chimera software. The binding sites between title molecule and 5P4Q protein are H9 and LIG (residue) and distance between H9-LIG is 2.169 Å. FF score and docking between title molecule and 5P4Q protein shows

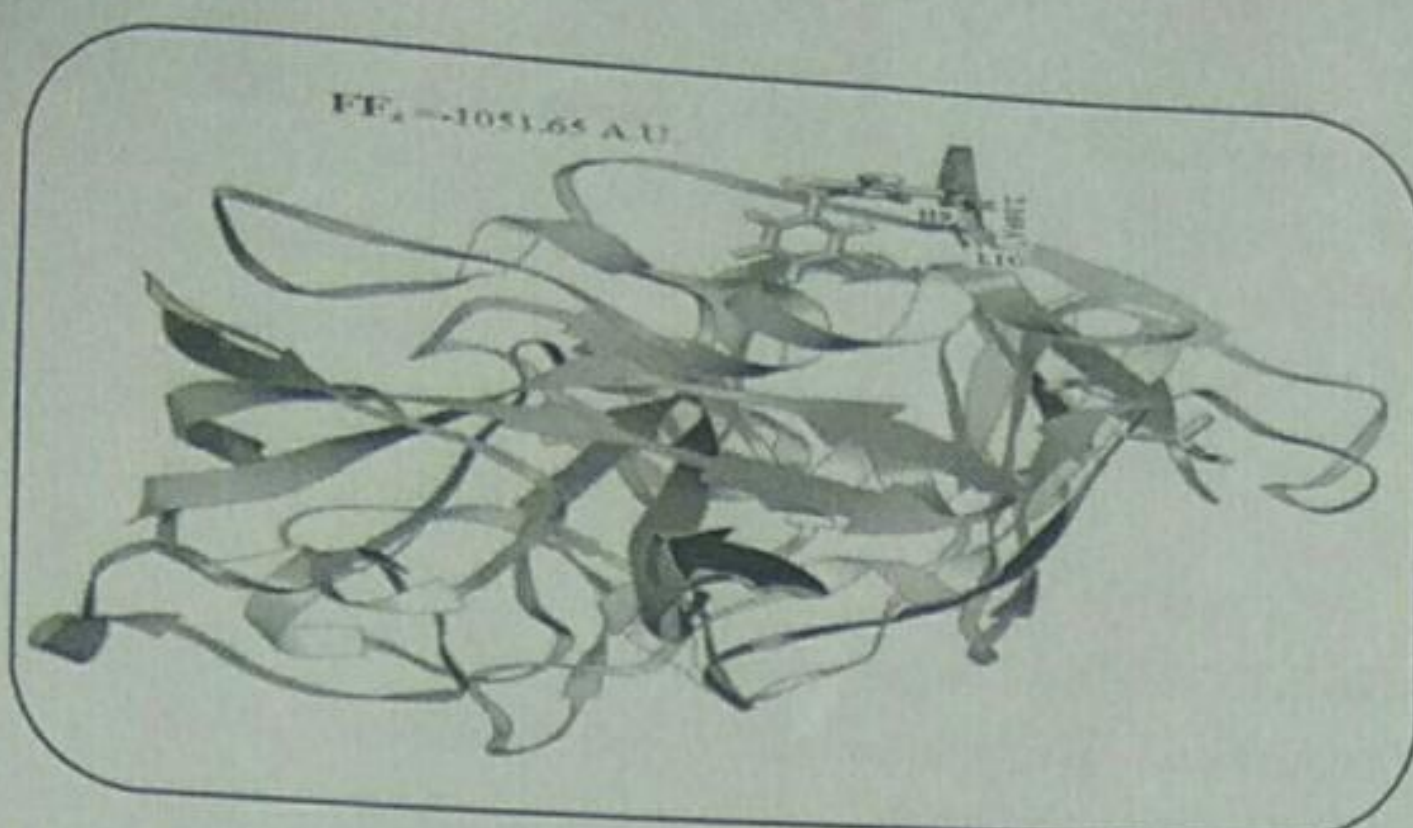


Fig. 8: Docking of Title molecule with 5P4Q protein predicated by Swiss Dock wave server.

that the molecule can be useful to stop fungus related diseases. This study gives a pathway for drug researcher to design new drugs for fungus related diseases.

CONCLUSIONS

In this paper we calculate geometric parameters, vibrational frequencies, electronic and the non-linear optical properties of title molecule using combination of DFT/B3LYP method and 6-311G (d, p) basis set. Optimized geometry clearly shows that the molecule is non-planar. Correlation factor > 0.99 between calculated and experimental value shows that they are well matched with each other. Non-linear optical behavior of the molecule shows that title molecule is optically active along the plane of the molecule. The molecular electrostatic potential contours and surfaces show that electron density transfer to benzene ring. NBO analysis shows that strongest interaction between bonding and antibonding orbitals is LP (1) N22 $\rightarrow \pi^*$ (C17-C20) with $E^{(2)}$ values 72.42 kcal/mol. The molecule shows better activity against allergic diseases.

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K. K. Kishor

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Kuntal Kishor

Health Amenities in Sitamarhi Municipality

Kuntal Kishor

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Abstract:

Health amenities are one of the most important basic needs of modern human civilization. It has been proved through various studies in developed and developing countries that health facilities not only insures better health of the resident population but also drops fertility rate and enhance economic growth. In this research article author has found out the condition of health amenities in Sitamarhi Municipality with etic and emic approach. The first approach of the study is based on the data of available health amenities in the study area and second approach of the study is based on score of satisfaction of urban dwellers in the Municipality. Etic study of health amenities in Sitamarhi Municipality suggest that the health facilities in the town are average and need to be improved. On the other hand emic study of health amenities in the study area suggest that population of the study area is well satisfied with the health amenities they get. Conclusively it can be said that the town is inhabited mostly by first or second generation migrants, who do not get these facilities in their village. So, they are satisfied with poor health facilities in the town.

Key words: Amenities, fertility rate, economic development, etic, emic, migrants

Introduction: Health Amenities

Medical revolution in western world and diffusion of their innovative medical technologies in third world countries has gradually changed the health condition of world population. Mortality rate has substantially reduced after medical revolution and fertility rate is decreasing fast even in developing countries. R. P. Mishra (1969) writes "Poor health makes the people less productive. Less production means less income which in turns means increased poverty". So medical revolution in 1960s not only made people healthy but also wealthy. Better health facility in any region/ country ensures high economic development and vice versa. Welfare governments have different policies for development of health facilities for the population. Ayushman Bharat yojana (25 September, 2018) of Indian Government is world's largest health insurance scheme. India spends 1 percent of GDP for health facilities. (Times of India, New Delhi, 20 June 2018).

Health facilities include Hospitals and clinics, Drug manufacturing units and distribution outlets, drug research and development centers and health education. At the public end Hospitals and medical clinics, and drug outlets are the basic health amenities. State and Central Government together with Urban Local Bodies (ULBs) are equally responsible for provision and distribution of amenities in municipalities.

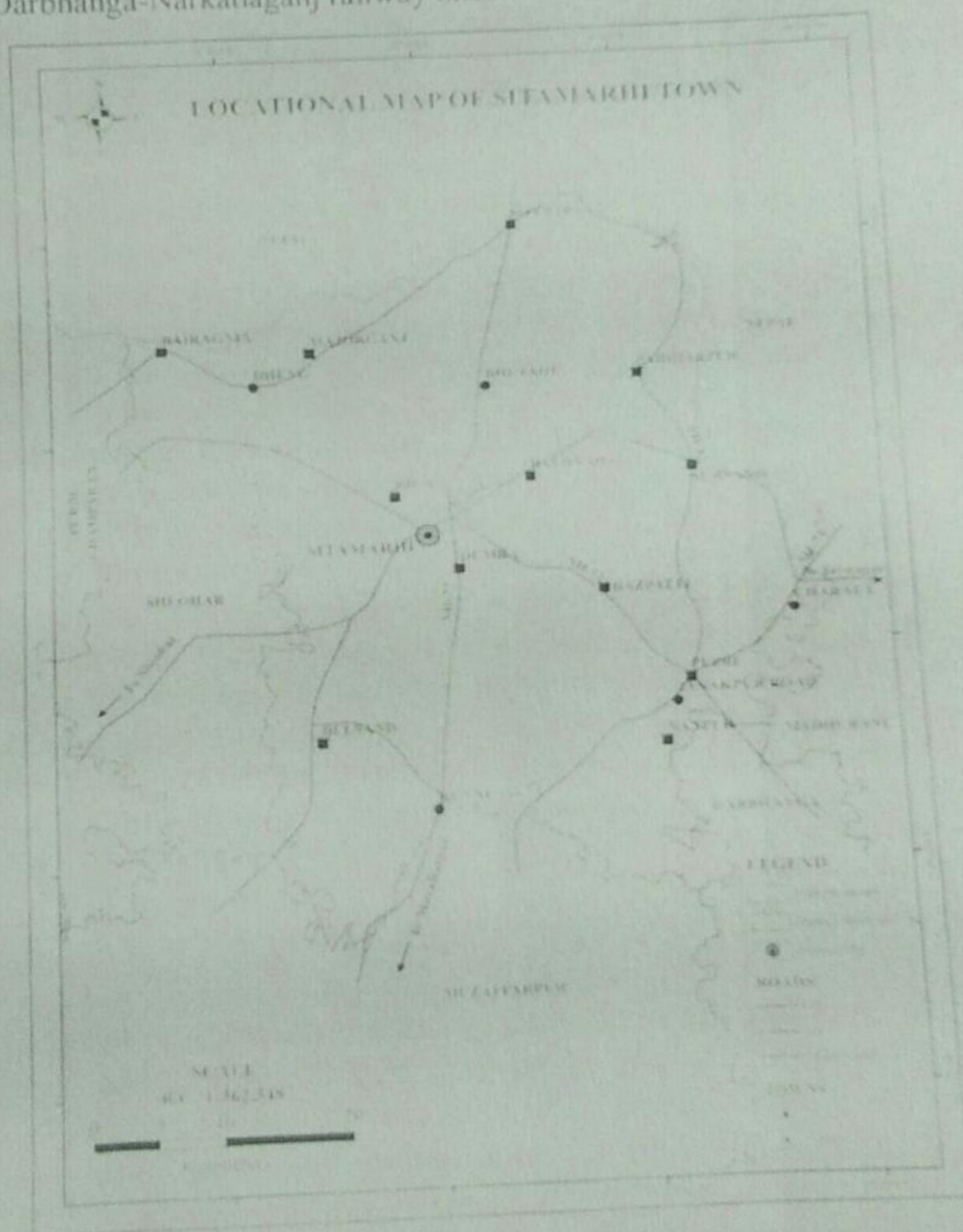
Study Area: Sitamarhi Municipality

Sitamarhi Municipality is situated in Northern Ganga Plain geographical region. It is a small town of Bihar. The town Sitamarhi is administrative unit (municipal council) of Dumra block and situated in the center of the block. National Highway 77 connects it to Muzaffarpur and Patna district to the South. State highways link it to Madhubani district in the east and Sheohar district in the west. The town Sitamarhi is situated on the Darbhanga-Narkatiaganj railway line and has the largest railway station

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of the district. There is another broad gauge track, running between Muzaffarpur and Sitamarhi. Sitamarhi municipality was constructed in 1882 and had a municipal board consisting of 12 commissioners. At that time there were only 4 wards in the town (Bihar District Gazetteers Muzaffarpur, 1958). Now the municipality is divided into 28 wards. As a sequel to the great earthquake in 1934 district court was shifted to Dumara (in 1936) located at 5 km south of Sitamarhi town. Dumara Notified Town Area Committee was constituted in 1937. Sitamarhi urban agglomeration occupies Dumara Notified Town Area as a statutory town. At present most of the government offices of Sitamarhi district are situated in Dumara.

The study area, Sitamarhi municipal council is situated almost in the center of Sitamarhi district, within Dumara block and occupies an area of about 5 square kilometer. The shape of Sitamarhi municipal council (SMC) is almost rectangular. The SMC has maximum east-west extension of 4.5 km and maximum north-south extension of 3 km. The site of the town Sitamarhi is a flood free site on natural levee of river Lakhandei. The municipal council has rivarian situation on both side of the river Lakhandei and has an important location at the confluence of state highway and NH 77, and along Darbhanga-Narkatiaganj railway line.



K. K. Kishor

Research Problem:

Research problem is an interrogative statement about relationship between different variables in the study area. To examine the condition of health amenities in Sitamarhi Municipality, researcher has formulated following research problems:

1. Is there any spatial variation in provision of health amenities?
2. Are the urbanites satisfied with the health amenities provided to them?

This research paper tries to find out the relationships; between geographical location and provision of health amenities, between provision of health amenities and degree of satisfaction of urbanites.

Objective:

Objectives of this study are:

1. To assess the condition of health amenities in different wards of Sitamarhi Town.
2. To find out spatial variation in provision of health amenities in the town.
3. To find out the degree of satisfaction of urbanites with health services.

Methodology:

The *etic* approach to find out the condition of health amenities in the study area includes collection of data regarding available health services in the town. For this purpose primary data from the town and secondary data of census survey (2011) have been collected by the investigator. The *emic* approach to find out condition of health amenities in Sitamarhi Municipality incorporates the assessment of satisfaction of urbanites with the health amenities provided to them. During execution of this research the investigator has collected primary data from twenty respondents from each wards of the town. This data represent the score of satisfaction with health amenities. Respondents were asked to give the score (1 to 5) to the health facilities they get in the town. Total score of satisfaction with different amenities in different wards of Sitamarhi Municipality has been calculated by adding individual score of satisfaction. On the basis of these composite scores of satisfaction with various amenities in every ward of the town, overall condition of urban amenities in Sitamarhi town and spatial variation in provision of urban amenities has been assessed.

Limitation of Methodology: This study is based on the data regarding level of satisfaction of the respondents. The satisfaction level of the respondent depends on their background (mental construct). People who have come from rural background are more satisfied with the facilities they get but on the other hand people with urban background feel these services in poor condition. So, this study is highly variable with people's background. In spite of this limitation this method is the most suitable way to study urban amenities, because people's appreciation is the most important factor for a service to become an amenity.

Findings: Medical Amenities

Sitamarhi town was frequently attached by epidemics like Cholera, Malaria and Chicken Pox before 1970s but the progress in sanitation and sewerage facility and better medical facilities has substantially reduced these microbial epidemics. The town has one Hospital at district level (Zila Aspatal) known as Sadar Hospital, Sitamarhi near Ramkrishna Goenka College. There is one PHC in Dumra, nearly 5 km from the main town where people from southern and Southwestern part of the town go for medical treatment. These two government Medical Centers are assisted by numerous private clinics and hospitals.

Table 1
Health facilities in government hospitals, Sitamarhi (M), 2016

Hospital	Facilities	Quantitative/Qualitative Information
Sitamarhi Hospital	Number of Bed	80 (available) 500 (sanctioned)
	Number of Doctors	13 (sanctioned) 13 (available)
	Number of Nursing Staff	29 (sanctioned) 29 (available)
	Number of other Staff	6
	Available Test Facilities	TLC, DLC, FNAC, Lipid Profile, Semen, Urine, Biopsy, BUN, Blood Sugar, SGPT, Culture, SGOG, X-ray, Ultrasound
	Departments	General Medicine, Surgery, Orthopedics, Gynaecology, Pediatrics, ENT, Dentistry, Diabetese ART, Dermatology, ANC Tuberculosis
PHC, Dumara	Number of Bed	NA
	Number of Doctors	3 (sanctioned) 2 (available)
	Number of Nursing Staff	26 (sanctioned) 26 (available)
	Number of other staff	4
	Available test facility	TLC, DLC, Lipid profile, Semen, Urine Blood Sugar, SGPT, Culture, X-ray, Ultrasound
	Departments	General Medicine, Surgery, Malaria, Tuberculosis, Gynecology
	Ambulance	1

Source: District census handbook, Sitamarhi, series-11, part B, 2011

Several other functions like Immunization Camp, blood collection camp, Blood Sugar test Camp etc. are organized by Sadar hospital and Dumara PHC. These camps are very productive and task oriented having more than expected success rate. The town has many Private Hospital and clinics. Some of these are listed in tables above. Almost all facilities related to health and immunization is available in these hospitals.

Table 2
Private Hospitals in Sitamarhi town (2016)

Name of Hospital	Number of bed
Ashirwad Hospital	25
Nandipant Hospital	15
Renu Singh Clinic	75
Dr. Anju Singh Hospital	40
Dr. Lata Gupta Hospital	30

Dr. Lata Gupta

Hospital Gunja	25
S P. Jha Hospital	20
Suresh Bawesh Clinic	25
Sukhsagar Hospital	25

Source: Information collected through field survey (2015-16)

Table 3

Composite score of satisfaction with medical facility in Sitamarhi(M)

Ward Number	Total respondent	Score given by respondents (out of 5)						Total score		
		5		4		3			2	
		1	0	1	0	1	0		1	0
1	20	3	9	7	1	0	0	74		
2	20	3	8	6	2	1	0	70		
3	20	4	8	6	2	0	0	74		
4	20	3	9	7	1	0	0	74		
5	20	2	8	10	0	0	0	72		
6	20	4	8	8	0	0	0	76		
7	20	3	9	8	0	0	0	75		
8	20	5	10	4	1	0	0	79		
9	20	2	9	8	1	0	0	72		
10	20	5	10	5	0	0	0	80		
11	20	4	8	6	2	0	0	74		
12	20	2	8	9	1	0	0	71		
13	20	3	8	8	1	0	0	73		
14	20	3	7	8	2	0	0	71		
15	20	2	9	8	1	0	0	72		
16	20	4	10	6	0	0	0	78		
17	20	6	11	3	0	0	0	83		
18	20	5	10	5	0	0	0	80		
19	20	6	10	4	0	0	0	82		
20	20	4	9	7	0	0	0	77		
21	20	3	8	8	1	0	0	73		
22	20	3	9	7	1	0	0	74		
23	20	5	11	4	0	0	0	81		
24	20	2	8	6	4	0	0	68		
25	20	2	7	10	1	0	0	70		
26	20	2	8	9	1	0	0	71		
27	20	4	10	4	2	0	0	76		
28	20	7	11	2	0	0	0	85		

Source: Field survey (2016)

The data related to degree of satisfaction with the medical facility in the town shows that population living in ward number 10,17,18,19 and 23 are more satisfied with the facility than residents of other wards. It means medical facility in these wards is more satisfactory than in other wards.

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Conclusion:

Etic study of health amenities in Sitamarhi Municipality suggest that the health facilities in the town are average and need to be improved. On the other hand emic study of health amenities in the study area suggest that population of the study area is well satisfied with the health amenities they get. Conclusively it can be said that the town is inhabited mostly by first or second generation migrants, who do not get these facilities in their village. So, they are satisfied with poor health facilities in the town.

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Full Length Article

Structural, IR spectra NBO, TDDFT, AIM calculation, biological activity and docking property of [1,2,4]-triazolo[3,4-*b*][1,3,4] thiadiazoleAnoop Kumar Pandey^a, Dharmesh Vikram Shukla^b, Vijay Singh^c, Vijay Narayan^{d,*}^a Govt. College Bishrampur Surajpur (C.G.), India^b GLA University Mathura (C.G.), India^c The University of Dodoma, Dodoma, Tanzania^d S.R.M.G.P.C., Lucknow, India

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ABSTRACT

In this paper a complete quantum chemical study of [1,2,4]-triazolo [3,4-*b*][1,3,4] thiadiazole has been done with the combination of DFT/B3LYP method and 6-311G(d, p) basis set. The vibrational assignments are calculated with the help of PED. By using quantum theory of atoms in the molecule (QTAIM) we have calculated topological parameters at BCP point by which the nature of several intermolecular hydrogen bondings are studied. Electronic properties are calculated with the help of HOMO-LUMO plot. Chemical active sites of title molecule are described by FF, chemical hardness, chemical softness etc. UV spectra are calculated with the help of TDDFT using optimized parameters. NBO analysis gives idea about transfer of charge between bonding and antibonding electrons. Biological activity analysis suggests that the molecule can be used in anti-inflammatory drugs to explore new drugs. The molecule is docked with MBNL1 receptor with the help of Swiss-Dock online server with Full fitness score of -541.58 a.u.

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1. Introduction

1,3-thiazole containing both Nitrogen and sulphur is a heterocyclic compound. The term 'thiazole' refers to a large family of derivatives [1]. Thiazole having molecular formula C_3H_3NS is a soft yellow liquid with pyridine-like scent [2] and used in a variety of specialized products, often by fusing with benzene derivatives. These are naturally occurring peptides, and utilized in the commercial development of peptidomimetics [3,4]. Thiazole is heterocyclic series organic compound characterized by a ring structure composed of three carbon atoms, one nitrogen atom, and one sulphur atom. This ring structure attributes many significant biologically active natural qualities such as thiamine, penicillin, and in many synthetic drugs, dyes, and industrial chemicals [5,6]. These are found in a number of various food products and flavors and are used in the manufacturing of prepackaged food products including noodles [7]. Thiazoles help flavorists to create healthier crops by enhancing the flavor of meats and savory foods without

the accumulation of excess salts or fats [8]. 1,2,4-Triazole derivatives and their bonded heterocyclic correspondents are well known for their different biological activities and 1,2,4-triazole rings have been combined into ligands used in coordination compounds. The 1,2,4-triazole derivatives and their *N* bridged heterocyclic equivalents have been widely studied [9–14]. Numerous 3,6-disubstituted [1,2,4] triazole [3,4-*b*] [1,3,4] thiadiazoles are testified to display significant antibacterial [15–18], pesticidal [19], anticancerous [20], anti-inflammatory, and anti-oxidant activities [21]. Many studies are carried to synthesize organic compounds, inorganic metal complexes and are detected by using NMR FTIR spectra [22–27]. Monirah A. Al-Alshaikh et al. synthesized the crystal structure of [1,2,4]-triazolo[3,4-*b*][1,3,4] thiadiazole molecule and found it as a potential bioactive agent [22–28]. The present study on the [1,2,4]-triazolo[3,4-*b*][1,3,4] thiadiazole molecule has been carried out to support and as an extension of the work of Monirah A. Al-Alshaikh et al. [29]. As mentioned in the work of Monirah A. Al-Alshaikh et al., due to bioactive potential of the molecule its biological properties are studied by using several parameters and also docking is made for designing new anti-inflammatory drugs. Along with this the geometrical parameters, NMA, Biological and Chemical activities, electronic transitions,

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thermodynamic properties are studied by the combination of DFT/B3LYP method and 6-311G(d, p). A complete DFT analysis is performed on the title molecule (Fig. 1).

2. Computational details

All the calculations are done with G03 program package [29] using combination of B3LYP/DFT method and 6-311G (d, p) basis set. This basis set 6-311G (d, p), with 'p' polarization functions on hydrogen atoms and 'd' polarization functions on heavy atoms, is used for better description of polar bonds of molecule [30,31]. Initial geometry is modeled with the help of Gauss View 3.0 program package [32]. AIM calculation, performed by AIMALL program package [33], is based on quantum theory of atoms in a molecule. Natural bond analysis is carried with NBO 3.0 program package [34]. Electronic transitions, vertical excitation energies, and oscillator strengths are computed with the TD-DFT method.

3. Result and discussion

3.1. Optimized parameters

The molecule taken has two benzene rings, one thiazole and other phenyl rings. The molecule shows some deviation from planarity, with fluoro ring (C19-C14) forming dihedral angle of 2.65° and the phenyl ring (C12-N17) 3.84° . The distance of the interaction between benzene ring and thiazole ring C14-C19 is 2.33 Å.

AIM [35] calculation shows that there are two interactions between N18-H8 and N18-F29 in the molecule, which are shown in Fig. 2. According to Koch and Popelier standard, an existence of hydrogen bond follows bond critical point (BCP) for the 'proton (H)...acceptor (A)', [36] which involves electron density (ρ) in the range of 0.002–0.040 a.u. and Laplacian ($\nabla^2\rho$) in the of range 0.024–0.139 a.u. All calculated parameters at BCP, in between N18-H8, and N18-F29, are listed in Table 1. On the basis of topological parameters three types of H-bonds are characterized. According to Rendering to Rozas et al. [37], the characterization demands, at BCP, that for strong and covalent nature of H-bond $\nabla^2\rho < 0$ and $H < 0$, for medium and partially covalent nature of H-bond $\nabla^2\rho > 0$ and $H < 0$, and for weak H-bond of electrostatic character $\nabla^2\rho > 0$ and $H > 0$. From Table 1, the Laplacian of charge density are positive, however value of $H < 0$ signifies that the interaction is medium strong in nature. According to Espinosa et al. interaction energy calculated is $E_{\text{int}} = \frac{1}{2} V$ at BCP [38]. In this study calculated interaction energy of N18-H8, N18-F9 is 3.95 kcal/mol and 5.648 kcal/mol respectively.

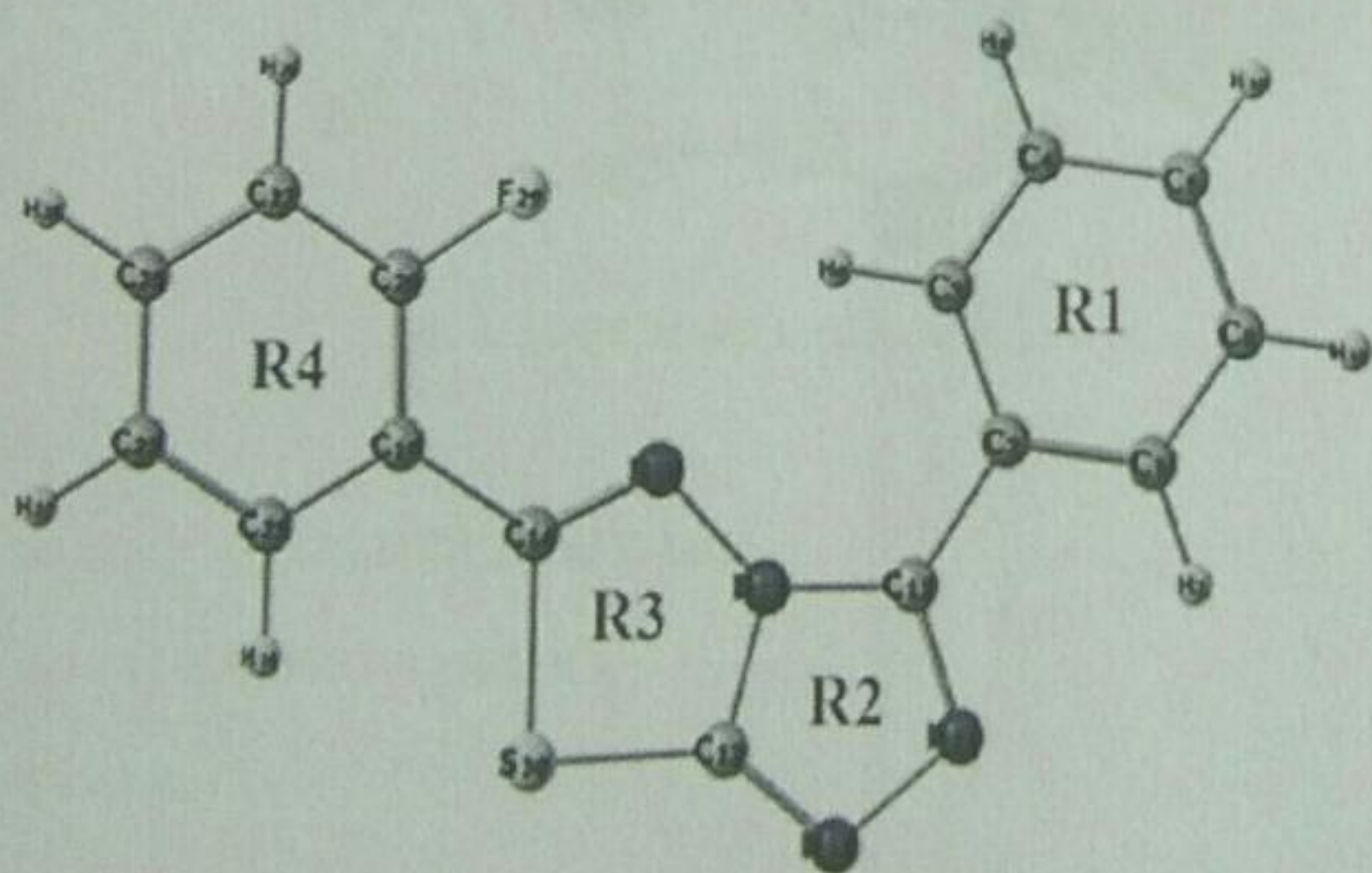


Fig 1. Molecular Picture of title molecule according to numbering.

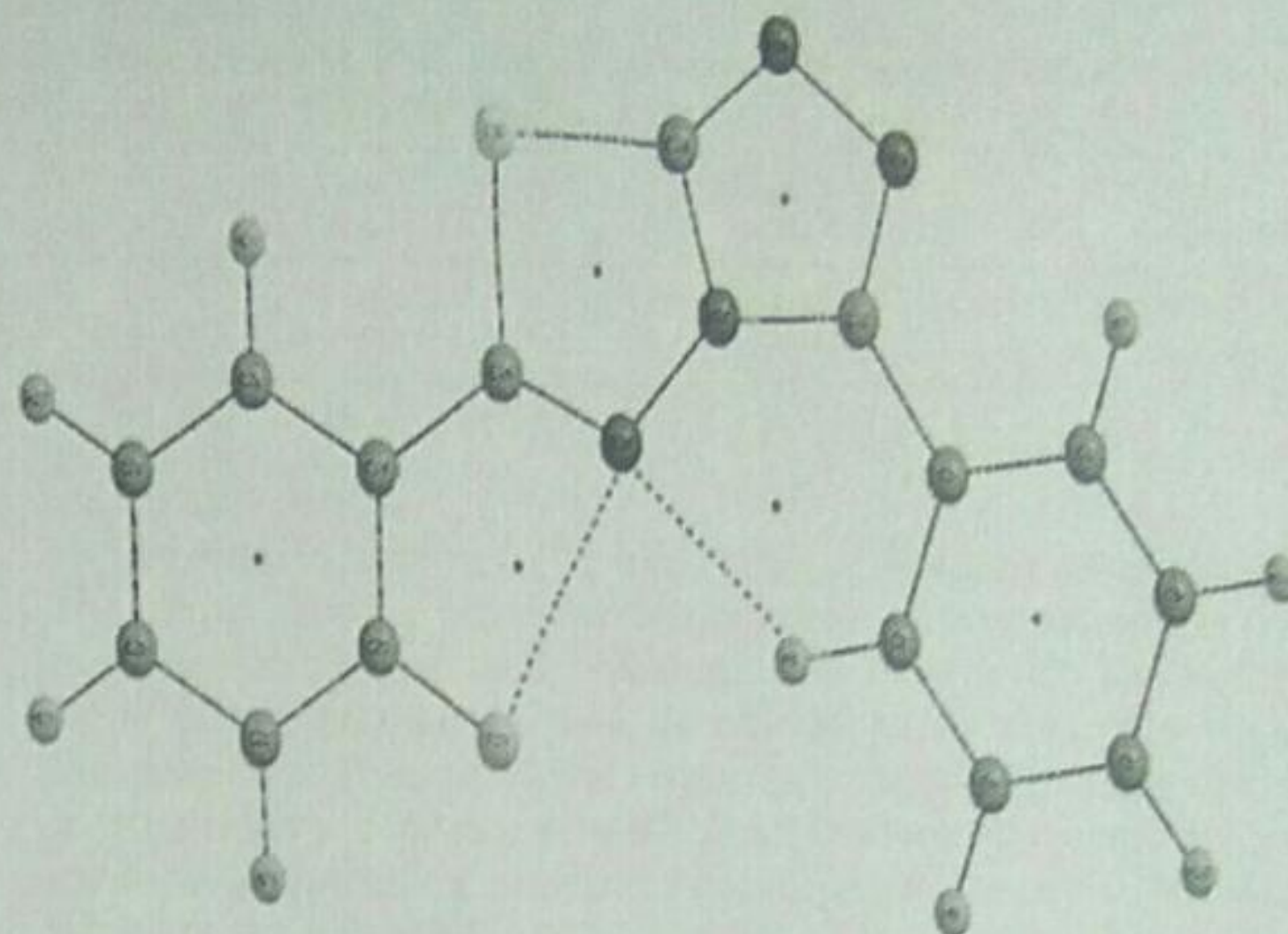


Fig 2. Molecular Graph of the studied compound at BCP.

3.2. Electronic property and HOMO-LUMO surfaces

The HOMO represents the ability to donate an electron by an atom while LUMO represents the ability to accept. The HOMO and LUMO energies are calculated by DFT/B3LYP method. The electronic parameters, such as highest occupied molecular orbital (HOMO) energy (E-HOMO), lowest unoccupied molecular orbital (LUMO) energy (E-LUMO) and band gap energy ($\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$) are described theoretically [39]. The energy (E_{gap}) between HOMO and LUMO in the present study is found to be 3.71 eV. In this molecule LUMO is located over whole molecule however HOMO is located only on benzene ring. The transition from HOMO \rightarrow LUMO in the molecule indicates charge transfer from benzene ring to thiazole ring. The molecular electrostatic potential (MESP) is a map of potential i.e. electrostatic potential over constant electron density of all molecules. It displays molecular size and shape as well as positive, negative, and neutral electrostatic potential regions in terms of color grading scheme. In this color grading schemes, the blue color represents the most electropositivity i.e. low electron region, whereas the red color corresponds to the most electronegative center or electron rich regions [40,41]. The MESP plot of title molecule is display in Fig. 3. From this fig. ring R₂ is covered by red region so it is the most electronegative region of title molecule. On the basis of energy of frontier orbitals, ϵ_{HOMO} , ϵ_{LUMO} [energy of highest occupied molecular orbital, Energy of lowest unoccupied molecular orbital respectively] the different global reactivity descriptors such as electronegativity χ (tendency to attract electrons), chemical potential μ (energy that can be absorbed or released), global hardness η (hardness basically signifies the resistance against the deformation or polarization of the electron cloud of the atoms, ions or molecules under small perturbation of chemical response), global electrophilicity index ω (capacity of a species to accept arbitrary number of electrons) and global softness S (Softness signify how easily a molecule becomes polarized) are computed using equations as given below [42] (Fig. 4).

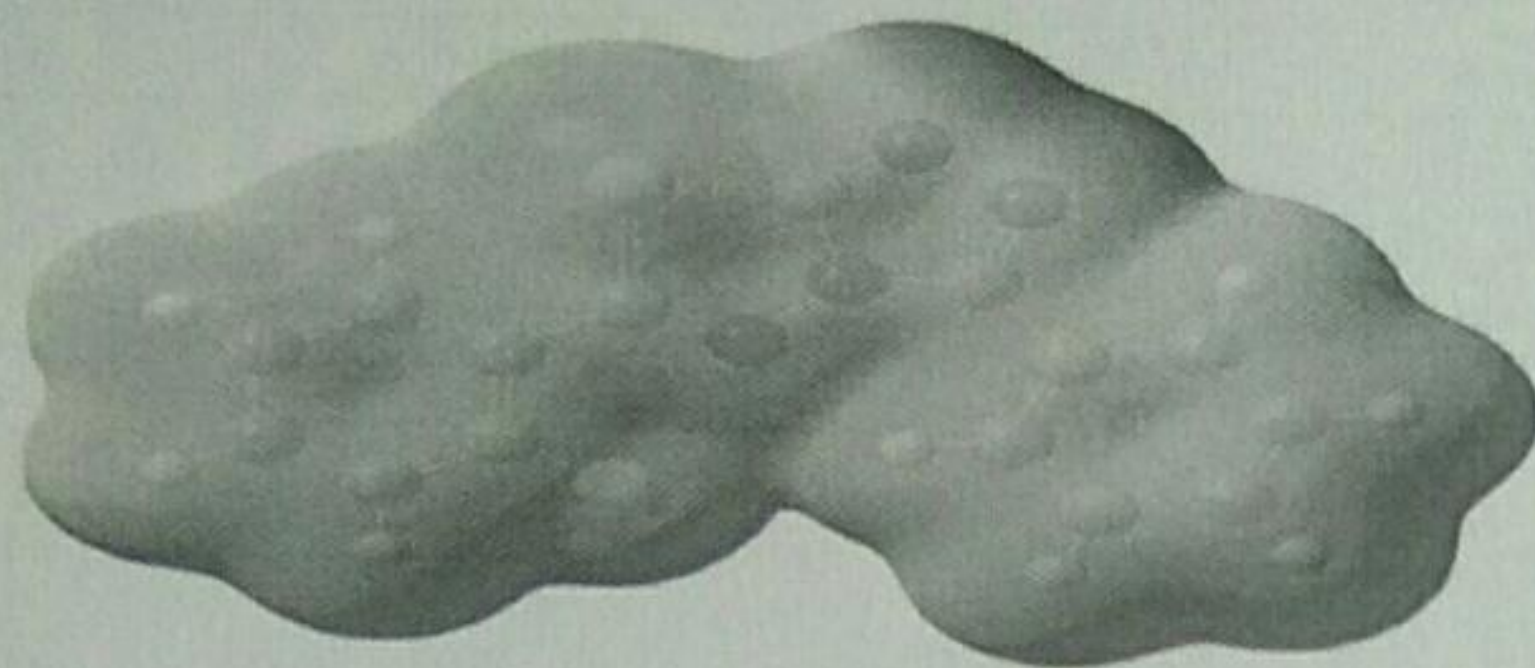
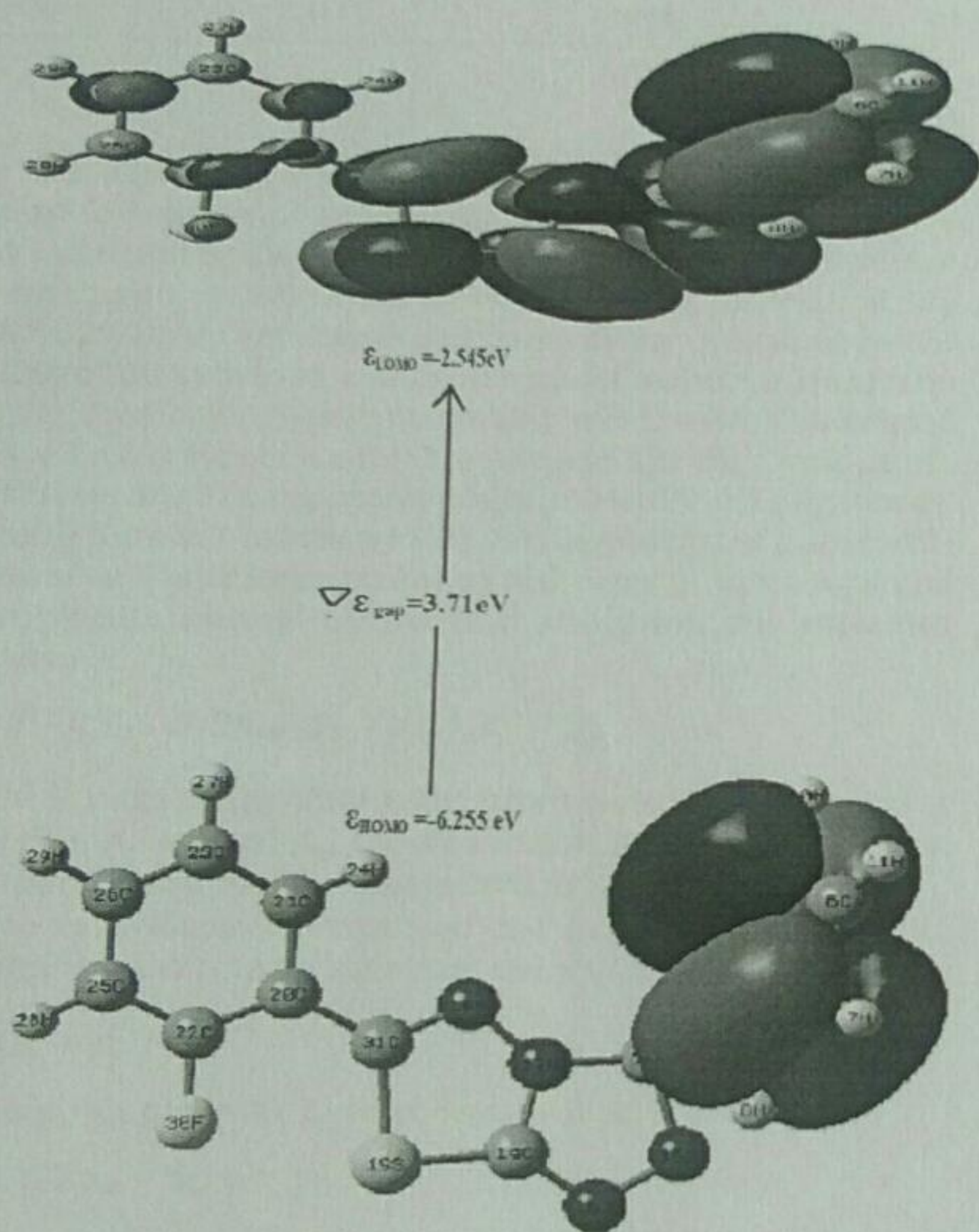
The energies of frontier molecular orbitals (ϵ_{HOMO} , ϵ_{LUMO}), energy band gap ($\epsilon_{\text{LUMO}} - \epsilon_{\text{HOMO}}$), electronegativity (χ), chemical potential (μ), global hardness (η), global softness (S), and global electrophilicity index (ω) of the molecule have been listed in Table 2. On the basis of ϵ_{HOMO} and ϵ_{LUMO} , these parameters are calculated by using equation given below [43–45]

$$\chi = -1/2(\epsilon_{\text{LUMO}} + \epsilon_{\text{HOMO}})$$

Table 1

Topological parameters for bonds of interacting atoms: electron density (ρ_{BCP}), Laplacian of electron density ($\nabla^2 \rho_{\text{BCP}}$), kinetic electron energy density (G_{BCP}), potential electron energy density (V_{BCP}), total electron energy density (H_{BCP}), estimated interaction energy (E_{int}) at bond critical point (BCP).

O–H	ρ_{BCP} (a.u.)	$\nabla^2 \rho_{\text{BCP}}$ (a.u.)	G_{BCP} (a.u.)	V_{BCP} (a.u.)	H_{BCP} (a.u.)	E_{int} (kcal/mol)
N18–H8	0.0150	0.0630	0.0142	–0.013	–0.014	3.953
N18–F29	0.0159	0.0897	0.0201	–0.018	–0.0186	5.648

**Fig. 3.** MESP surfaces of thiazol.**Fig. 4.** HOMO, LUMO surfaces of thiazol.

$$\mu = -\chi = 1/2(\epsilon_{\text{LUMO}} + \epsilon_{\text{HOMO}})$$

$$\eta = 1/2(\epsilon_{\text{LUMO}} - \epsilon_{\text{HOMO}})$$

$$S = 1/2\eta$$

$$\omega = \mu^2/2\eta$$

3.2.1. Fukui function

The Fukui function (FF) [46,47] of a molecule provides information about reactive sites and the method of understanding as well as categorizing chemical reactions. The atom with the highest FF value is highly reactive site as compared to the other atoms in the molecule. The use of the Fukui functions for the site selectivity in title molecule for nucleophilic and electrophilic attacks has been made with special emphasis on the dependence of the Fukui values with the basis of B3LYP/6-311G(d, p) level of theory. Using the Mullikan atomic charges of neutral, cation, and anion, state of the molecule, the Fukui functions (f_k^+ , f_k^- , f_k^0), local softness (S_k^+ , S_k^- , S_k^0) [48] and local electrophilicity indices (ω_k^+ , ω_k^- , ω_k^0) are calculated using the following equations

$$f_k^+ = [q_k(N+1) - q_k(N)] \text{ for nucleophilic attack}$$

$$f_k^- = [q_k(N) - q_k(N-1)] \text{ for electrophilic attack}$$

$$f_k^0 = 1/2[q_k(N+1) + q_k(N-1)] \text{ for radical attack.}$$

where q_k is electronic population of atom k in the neutral molecule with N electrons.

Local softness and electrophilicity indices are calculated using

$$S_k^\pm = S f_k^\pm, \quad S_k^0 = S f_k^0, \quad \omega_k^\pm = \omega f_k^\pm, \quad \omega_k^0 = \omega f_k^0$$

where +, –, and 0 signs show nucleophilics, electrophilics, and radical attacks, respectively. The Fukui functions, for all the carbon atoms in both benzene ring (R_1 – R_4) and sulfur atom in thiazole ring (R_3), calculated by using combination of DFT/B3LYP method and 6-311G (d, p) basis set are listed in Table 3. From Table 3, it can be seen that the carbon of both benzene ring, 14C and 31C are more reactive sites for nucleophilic and 26C as an electrophilic reactive attacks. However 30S atom of the thiazole ring shows more favorable site for both electrophilic and nucleophilic substitution than ring carbon atoms. Furthermore, 30S site is more reactive to the electrophilic than nucleophilic substitution because $f_k^- > f_k^+$.

Time dependent density functional theory (TD-DFT) method is important tool for studying the nature of the transitions of UV–vis spectrum of the compound. Optimized geometry is obtained for TD-DFT calculation by using same level theory. UV spectra of the molecule, calculated by combination of DFT/B3LYP method and 6-311G (d, p) basis set is shown in Fig. 6. In this graph, two prominent peaks observed at 4.02 eV (294 nm), 2.03 eV (610 nm) originate mainly due to $H \rightarrow L$ (37%), $H-4 \rightarrow L$ (43%) transitions respectively. These transitions are shown in Fig. 5 and listed in Table 4. On the basis of the calculated molecular orbital coefficients analyses electronic transition are assigned to $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ respectively.

3.3. Non linear optical parameter

The Gaussian 03 program is used to calculate the dipole moment (μ) and polarizability (α) of the molecules, based on the finite field approach. The first hyperpolarizability (β) and polarizability of the title molecule are calculated by using same level the-

Table 2

Electronic parameters of title compound calculated by DFT/B3LYP method and 6-311G(d, p).

HOMO energy	LUMO energy	Electronegativity (χ)	Chemical potential (μ)	Global hardness (η)	Global softness (S)	Global electrophilicity index (ω)
-6.255	-2.545	4.400	-4.400	1.855	0.270	5.218

Table 3

Fukui values on the basis theory of the Mulliken atomic charges of neutral, cation, and anion, the Fukui functions (f_k^+ , f_k^- , f_k^0).

S.N	Neutral	Positive	Negative	f_k^+	f_k^-	f_k^0
1C	-0.133	-0.128	-0.136	0.005	0.003	-0.132
2C	-0.171	-0.173	-0.163	-0.002	-0.008	-0.168
3C	0.188	0.190	0.191	0.002	-0.003	0.191
4C	-0.171	-0.169	-0.169	0.002	-0.002	-0.169
5C	-0.133	-0.129	-0.135	0.004	0.002	-0.132
6C	-0.123	-0.113	-0.129	0.010	0.006	-0.121
12C	0.041	-0.011	0.077	-0.052	-0.036	0.033
14C	0.313	0.344	0.239	0.031	0.074	0.292
20C	0.069	0.063	0.070	-0.006	-0.001	0.066
21C	-0.160	-0.147	-0.183	0.013	0.023	-0.165
22C	0.313	0.332	0.285	0.019	0.028	0.309
23C	-0.132	-0.126	-0.134	0.006	0.002	-0.130
25C	-0.190	-0.181	-0.199	0.009	0.009	-0.190
26C	-0.124	-0.105	-0.154	0.019	0.030	-0.130
31C	0.039	0.065	0.002	0.026	0.037	0.034
30S	0.301	0.484	0.118	0.183	0.183	0.301

ory and listed in Table 5. In the presence of applied electric field, energy is function of applied electric field. Hyperpolarizability and Polarizability are described as the response of a system due to application of the electric field [49]. The Hyperpolarizability and Polarizability are determined by nonlinear optical properties (NLO) of the system as well as strength of molecular interaction [50,51]. First order Hyperpolarizability of the system is defined by $3 \times 3 \times 3$ matrix of is a third rank tensor. The third rank matrix which contains 27 components can be reduced to 10 components by using Kleinman symmetry [52]. All components of β are coefficients in the Taylor series expansion of the energy. When weak and homogeneous external electric field is applied, this expansion becomes

$$E = E^0 - \mu_x F_x - 1/2 \alpha_{xx} F_x F_x - 1/6 \beta_{xxx} F_x F_x F_x$$

where E^0 is the energy of the unperturbed molecules, F_x the field at the origin μ_x , α_{xx} , and β_{xxx} are the components of dipole moment, polarizability and the first hyperpolarizabilities respectively.

The total dipole moment and the mean polarizability and hyperpolarizability using x,y,z components are defined as

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

where μ_x , μ_y , μ_z are X,Y,Z components of dipole moment

$$\langle \alpha \rangle = 1/3 [\alpha_{xx} + \alpha_{yy} + \alpha_{zz}]$$

where α_{xx} , α_{yy} , α_{zz} are the components of polarizability in XX, YY, ZZ planes

$$\beta_{Total} = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1/2}$$

$$= [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yxx} + \beta_{yzz})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2]^{1/2}$$

where β_{abc} are components of hyperpolarizability along a direction and in bc plane and (1 a.u. = 3.6998×10^{-30} e.s.u.).

The calculated value of dipole moment is 6.29 D. In title molecule α_{xx} and α_{yy} have greater contribution of polarizability which indicates that the molecule is more polarized along Y and X directions. The calculated value of hyperpolarizability of given molecule is

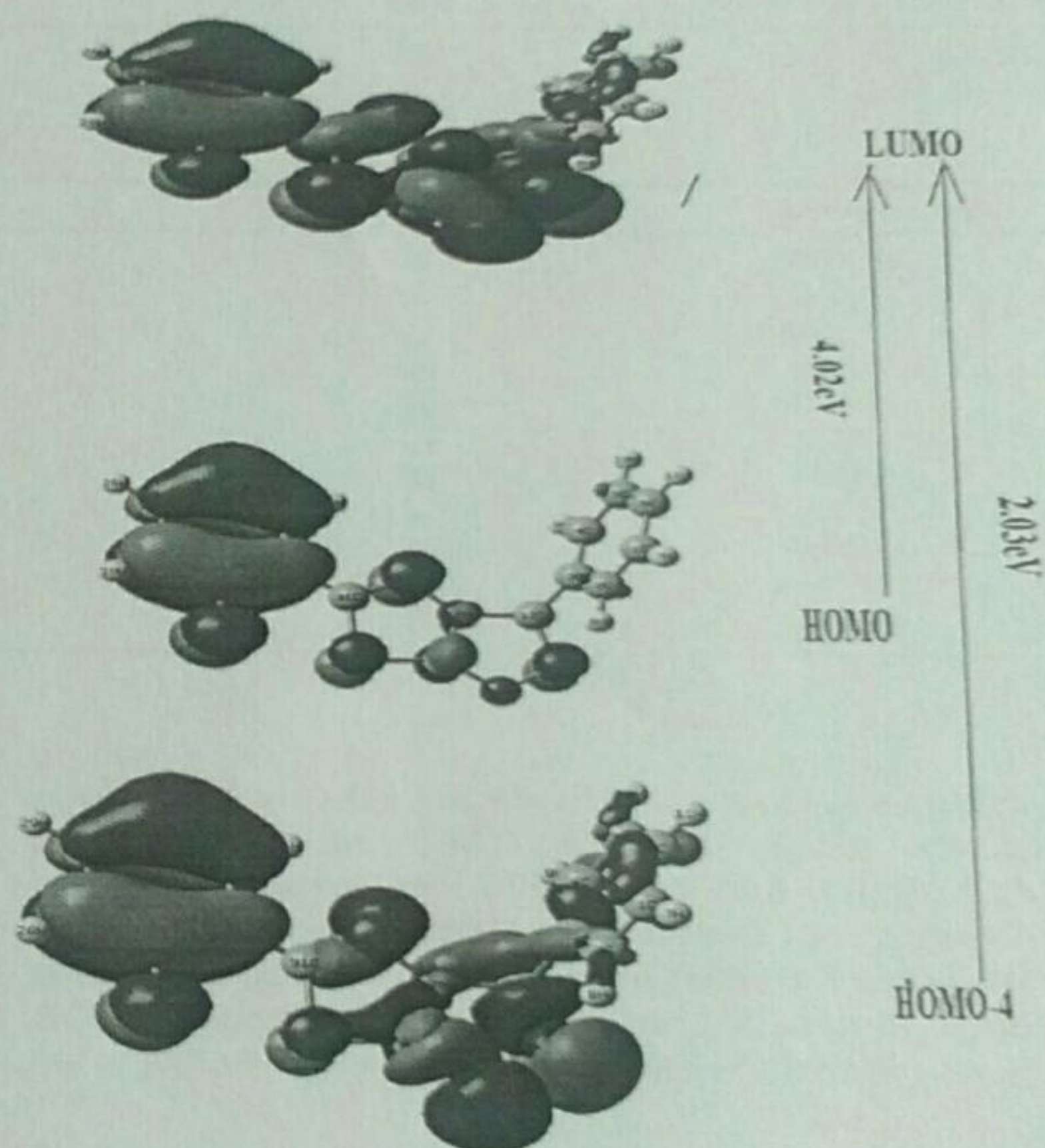


Fig 5. Electronic Transition of TD-DFT of title molecule by DFT/B3LYP method.

nearly same as, 2-[[5-(adamantan-1-yl)-4-methyl-4H-1,2,4-triazol-3-yl]sulfanyl]-N,N-dimethylethanamine [53], and nearly one fifth of Thiazole Azo Dyes.[54] Urea is benchmark compound for NLO properties, therefore we compare our results with urea. The calculated value of hyperpolarizability of the compound is nearly nine times greater than hyperpolarizability of urea so it is a good claimant as a NLO material.

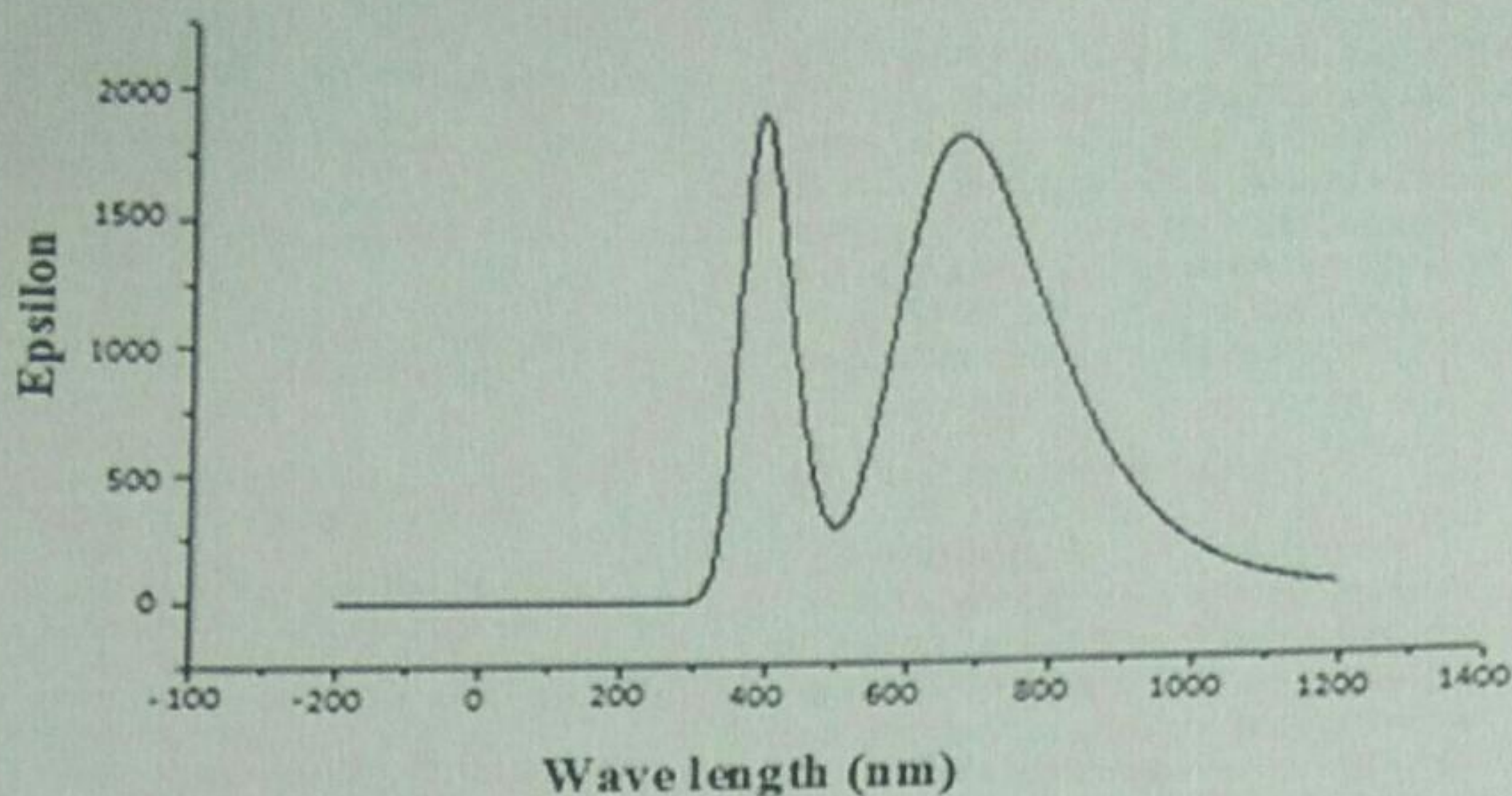


Fig 6. UV spectra of title molecule calculated by combination of DFT/B3LYP method and 6-311G(d,p) basis set.

Table 4

The observed UV-vis spectra as calculated by TD-DFT method at B3LYP/6-311 G (d, p) level.

Excitation energy (eV)	Wavelength (nm)		Oscillator strength	Orbital transition
	Calculated	Assignment		
4.02	294	$n \rightarrow \pi^*$	0.023	HOMO \rightarrow LUMO (43%)
2.03	610	$\pi \rightarrow \pi^*$	0.130	HOMO-4 \rightarrow LUMO (37%)

Table 5

Polarizability and Hyper Polarizability of title compound calculated by same level theory.

S.N.	Parameter	Polarizability	S.N.	Parameter	Hyper Polarizability
1.	α_{xx}	-113.889	1.	β_{xxx}	-130.786
2.	α_{yy}	-129.426	2.	β_{yyy}	58.531
3.	α_{zz}	0.393	3.	β_{zzz}	4.053
4.	α_{xy}	6.624	4.	β_{xyy}	-42.254
5.	α_{xz}	2.339	5.	β_{xxy}	77.013
6.	α_{yz}	-2.853	6.	β_{xxz}	35.379
7.	α	-9.678	7.	β_{xzz}	14.626
			8.	β_{yzz}	-1.132
			9.	β_{yyz}	-1.432
			10.	β_{xyz}	-1.856
			11.	β	211.201

3.4. Vibrational analysis

The molecule under study contains 30 atoms, so there are $3N-6$ modes of vibrations. All mode of vibration are studied with the help of combination of Gauss View and VEDA 4.0 program package [55]. In our calculations we ignore electron-electron correlation as well as an-harmonicity [56,57]. These approximations cause calculated frequencies to be in higher region than experimental results, therefore we scale calculated frequency by 0.9688. [58] Some of selected modes of vibrations are listed in Table 6 and calculated IR spectra of the molecule is also plotted in Fig. 7, using same level theory. Some important modes of vibrations are discussed below.

3.4.1. C-H stretching

The hetero aromatic structure shows the presence of C-H stretching vibrations in the region $2800-3100\text{ cm}^{-1}$ [58]. In the present study the C-H stretching vibration of the title compound is observed at $3066-3108\text{ cm}^{-1}$. Two sharp back to back peaks observed at 3077 cm^{-1} , 3076 cm^{-1} due to $\nu(\text{C-H})_{\text{R}_1}$ and mixing of $\nu(\text{C-H})_{\text{R}_1, \text{R}_4}$ with PED 24%, 43% respectively, are well matched with

experimental as well as calculated IR spectra of 2-(4-methoxyphenyl)benzo[d]thiazole at 3076 cm^{-1} [59]. An intense mixing of modes are observed at 1625 cm^{-1} due to $\beta(\text{CH})_{\text{R}_1}$ with PED 16%. In mid region of spectra very intense and sharp polarized peaks are observed at 1611 cm^{-1} and 1605 cm^{-1} due to $\beta(\text{CH})_{\text{R}_1}$, $\beta(\text{CH})_{\text{R}_4}$ respectively with PED 47% and 76%. In lower region some out of plane bending and twisting mode of vibrations occur.

3.4.2. C-N vibrations

The determination of C-N vibrations is a difficult task, because of the mixing of vibration in this region. Silverstein [58] has first time assigned C-N stretching absorption in the range of $1382-1266\text{ cm}^{-1}$. The C-N stretching vibration ($15\text{N}-12\text{C}$) and ($17\text{N}-12\text{C}$) in the molecule observed at 1266 cm^{-1} and 1263 cm^{-1} with PED contribution 15% and 46% respectively, are well matched (1267 cm^{-1}) with C-N stretching mode and lies in the same region as 2-(4-methoxyphenyl)benzo[d]thiazole [59]. In lower range of frequency some other in plane bending vibration modes ($14\text{C}-18\text{N}-17\text{N}$) and torsion ($14\text{C}-18\text{N}-17\text{N}-12\text{C}$) are obtained at 1088 cm^{-1} and 654 cm^{-1} respectively with PED contribution 20% and 79%.

Table 6
Theoretical (selected) vibrational wave numbers of title molecule using B3LYP/6-311G (d, p) and their assignment.

Cal. Freq. Sc. freq	IR Int.	Mode of vibration
3176	3077	22.26
3175	3076	4.35
3172	3073	33.69
3168	3069	4.36
3154	3056	3.89
3152	3054	3.89
3148	3050	9.39
1677	1625	540.56
1663	1611	581.20
1657	1605	34.93
1637	1586	40.23
1622	1571	52.34
1577	1528	14.89
1540	1492	19.68
1520	1473	14.30
1493	1446	0.12
1477	1431	150.32
1411	1367	29.25
1408	1364	34.13
1383	1340	2.43
1341	1299	9.29
1327	1286	3.30
1326	1285	3.24
1287	1247	10.02
1254	1215	150.36
1218	1180	15.79
1187	1150	64.61
1176	1139	0.26
1150	1114	15.86
1119	1084	5.45
1107	1072	0.73
1002	971	0.45
976	946	5.62
966	936	6.31
925	896	30.44
865	838	0.71
850	822	1.05
776	752	10.88
660	639	5.24
655	635	6.47
606	587	0.98
531	514	279.57
		R1[ν (1C-7H) (24%)]
		R1[ν (6C-11H) (24%)]
		R4[ν (26C-29H)] (27%) + R1[ν (1C-7H)] (16%]
		R1[ν (4C-9H) (47%) + ν (5C-10H) (26%)]
		R4[ν (25C-28H) (50%)]
		R1[ν (1C-7H) (49%)]
		R4[ν (21C-24H) (37%)] + R1[ν (6C-11H) (26%)]
		R1[β (2C-3C) (11%)] + R1[β (1C-2C) (14%)]
		R1[ν (2C-3C) (47%)]
		R4[β (24H-21C)(42%)] + R4[β (22H-23C) (34%)]
		R1[ν (1C-2C)](31%)] + R2[ν (15 N-12C) (11%)]
		R1[ν (1C-2C) (29%)] + R1[β (6C-11H)](34%)]
		R1[ν (5C-4C) (14%)] + R1[β (5C-4C-6C) (15%)]
		R1[β (1C-2C-3C) (14%)]
		R1[β (8H-2C) (17%)] + R4[β (21C-23C-26C) (21%)]
		R1[β (10H-5C-6C) (11%)] + R1[β (8H-2C-1C) (13%)]
		R1[ν (1C-2C) (27%)]
		R3[ν (14C-30S) (17%)]
		R1[ν (2C-3C) (15%)] + R1[β (8H-2C-1C) (21%)]
		R1[γ (3C-2C-1C) (21%)]
		R2[ν (14C-18N) (19%)] + R2[ν (15 N-12C) (13%)]
		R2[ν (12C-17N) (27%)] + R1[β (3C-6C-5C) (15%)]
		R2[ν (15N-12C) (39%)]
		R2[β (17N-12C-15N) (14%)] + R3[β (18N-14C-30S) (23%)]
		R1[ν (2C-3C) (18%)] + R2[β (12C-15N-16N) (13%)]
		R2[ν (17N-14C) (21%)] + R3[γ (14C-18N-17N) (19%)]
		R3[ν (14C-30S) (17%)] + R1[γ (11H-6C-5C) (23%)]
		R2[β (17N-12C-15N) (23%)] + R3[β (17N-14C-18N) (21%)]
		R4[γ (26C-23C-21C) (15%)] + R1[γ (1C-2C-3C) (21%)]
		R2[ν (15N-12C) (13%)] + R4[β (22C-29F) (42%)]
		R3[β (18N-14C-30S) (46%)] + R1[β (3C-2C-1C) (15%)]
		R2[β (17N-12C-15N) (12%)] + R1[β (1C-2C-3C) (11%)]
		R3[ν (30C-18N) (15%)]
		R4[τ (20C-21C-22C-23C) (24%)] + R3[τ (14C-17N-18N-30S) (21%)]
		R2[ν (15N-12C) (22%)]
		R4[τ (22C-23C-25C-26C) (11%)]+R2[τ (17N-12C-15N-16N) (10%)]
		R2[β (14C-17N-18N) (13%)]
		R1[τ (3C-6C-1C-2C) (11%)] + R3[τ (14C-17N-18N-30S) (15%)]
		R1[γ (6C-5C-4C) (11%)] + R2[γ (12C-15N-16N) (17%)]
		R1[τ (3C-6C-2C-1C) (24%)] + R3[τ (14C-18N-17N-13C) (18%)]
		R4[γ (19C-20C-22C) (17%)] + R1[γ (1C-2C-3C) (13%)]
		R3[τ (13C-17N-18N-30S) (30%)] + R1[τ (6C-5C-4C-3C) (42%)]

Abbreviations: β = in plane bending, γ = out of bending, ω = wagging, τ = twisting, S = scissoring, R = rocking, ν = stretching. Note: The PED distribution less than 12% are neglected for the sake of calculation.

3.4.3. C-C vibrations

Normally the (C-C) stretching vibrations are expected within the middle region of spectra. The C-C stretching vibrations of the aromatic compounds, calculated by B3LYP/6-311G (d, p) method, are at 1600 cm^{-1} , 1586 cm^{-1} , 1568 cm^{-1} , 1500 cm^{-1} and 1293 cm^{-1} in thiazole ring however in benzene ring C-C aromatic stretching mode of vibrations lies in between 1645 and 847 cm^{-1} . The other modes of vibration i.e. in-plane and out-of-plane bending are also observed at lower frequencies.

3.4.4. Other modes of vibration

Some other modes of vibrations are also reported at lower range of frequencies. In thiazole ring intense plane polarized mode of vibration due to ν (29F-20C) with PED 19% is obtained at 1207 cm^{-1} . In this study below 1000 cm^{-1} half segment of thiazole

ring experiences torsion τ (14C-17N-18N-30S) at 936 cm^{-1} with PED 21%, however opposite half segment of thiazole ring experiences very intense peak of torsion τ (29F-19C-22C-20C) at 520 cm^{-1} with PED 27%. In fuoro ring a medium intense polarized mode of vibration with polarization vector along the plane of ring, due to ν (29F-20C), is obtained at 1207 cm^{-1} with PED 15%. Some other modes of vibrations are reported in table however those mode of vibration are not reported for which PED < 15%.

3.5. Donor acceptor interaction

3.5.1. NBO analysis

NBO gives the most suitable 'natural Lewis structure' because all orbitals include the highest possible percentage of the electron density (ED). NBOs deliver an accurate method for studying intra and intermolecular interaction as well as charge transfer or conjugative interaction in different molecular systems [60]. The value of $E^{(2)}$ shows the strength of interaction in between electron donors and electron acceptors, i.e., As the value of $E^{(2)}$ increases the strength of interaction increases and vice-versa. For each donor NBO(i) and acceptor NBO(j), the strength of delocalization interaction (or stabilization energy) $E^{(2)}$ associated with electron delocalization between donor and acceptor is estimated by the second order energy lowering as [61,62]

$$E^{(2)} = \Delta E_{ij} = q_i \frac{F_{ij}^2}{\epsilon_i - \epsilon_j}$$

where q_i is the population of donor orbital or donor orbital occupancy; ϵ_i , ϵ_j are orbital energies (diagonal elements) of donor and acceptor NBO orbitals respectively; F_{ij} is the off-diagonal Fock or Kohn-Sham matrix element between i and j NBO orbitals. The second-order perturbation analysis of Fock matrix in NBO basis are listed in Table 7. From this table we see that strong intra-molecular hyper conjugative interactions are formed by orbital overlap $\text{Lp}(1)\text{N}15/\text{N}17, \text{Lp}(2)\text{S}30, \sigma(\text{C-C}), \sigma(\text{C-H}), \pi(\text{C-C}), \sigma^*(\text{C-C}), \sigma^*(\text{C-H}), \pi^*(\text{C-C})$ which results in intra-molecular charge transfer causing stabilization of the system. From Table 7, interactions between C1-C2 to C3-C4, C5-C6 of $\pi(\text{C1-C2}) \rightarrow \pi^*(\text{C3-C4})$ and $\pi(\text{C1-C2}) \rightarrow \pi^*(\text{C3-C4})$ with electron density 0.9897 e stabilize by 10.28 kcal/mol, 10.49 kcal/mol respectively. The interaction between C3-C4 to C1-C2, C4-C5, C12-C17 of $\pi(\text{C3-C4}) \rightarrow \pi^*(\text{C1-C2})$ $\pi(\text{C3-C4}) \rightarrow \pi^*(\text{C5-C4})$, $\pi(\text{C3-C4}) \rightarrow \sigma^*(\text{C12-C17})$ with electron density 0.833e stabilizes by 10.04 kcal/mol, 9.72 kcal/mol and 3.11 kcal/mole respectively. Similarly interaction between C5-C6 to C3-C4, C1-C2, of $\pi(\text{C5-C6}) \rightarrow \pi^*(\text{C3-C4})$ $\pi(\text{C5-C6}) \rightarrow \pi^*(\text{C1-C2})$ with electron density 0.829 e stabilizes by 9.6 kcal/mol, 10.54 kcal/mol respectively. A strong interaction observed in between lone pair $\text{Lp}(1)\text{N}17 \rightarrow \pi^*(\text{C14-N}18)$, $\pi^*(\text{N}18-\text{C}31)$ with energy 21.09 kcal/mol and 20.25 kcal/mol respectively are comparable with interaction has been observed due to the electron density transfer from the lone pair (LP1) of nitrogen atom to antibonding orbitals $\pi^*(\text{C-N})$ and $\pi^*(\text{N-C})$ with stabilization energies 41.07 and 46.78 kcal/mol, respectively in similar molecular system 2-[[5-(adamantan-1-yl)-4-methyl-4H-1,2,4-triazol-3-yl]sulfanyl]-N,N-dimethylethanamine [53]. Since π orbitals have lower occupancies than σ , correspondingly showing more electron- donating ability in comparison to σ orbital. This also shows that $[\text{Lp}(1)(\text{S}30) \rightarrow \pi^*(\text{C14-C16})]$ is the most intensive interaction between the acceptor and donor which results in the molecular stability. A very strong interaction by π^* to π^* orbital overlap of $\pi^*(\text{C}22-\text{C}25) \rightarrow \pi^*(\text{C}23-\text{C}26)$ stabilizes by 153.69 kcal/mol. In this system stabilization occurs by intermolecular interactions of orbital overlap among π and π^* orbitals, which results in intermolecular charge transfer (ICT). Since ICT makes molecule more polarized, it must be responsible for the NLO

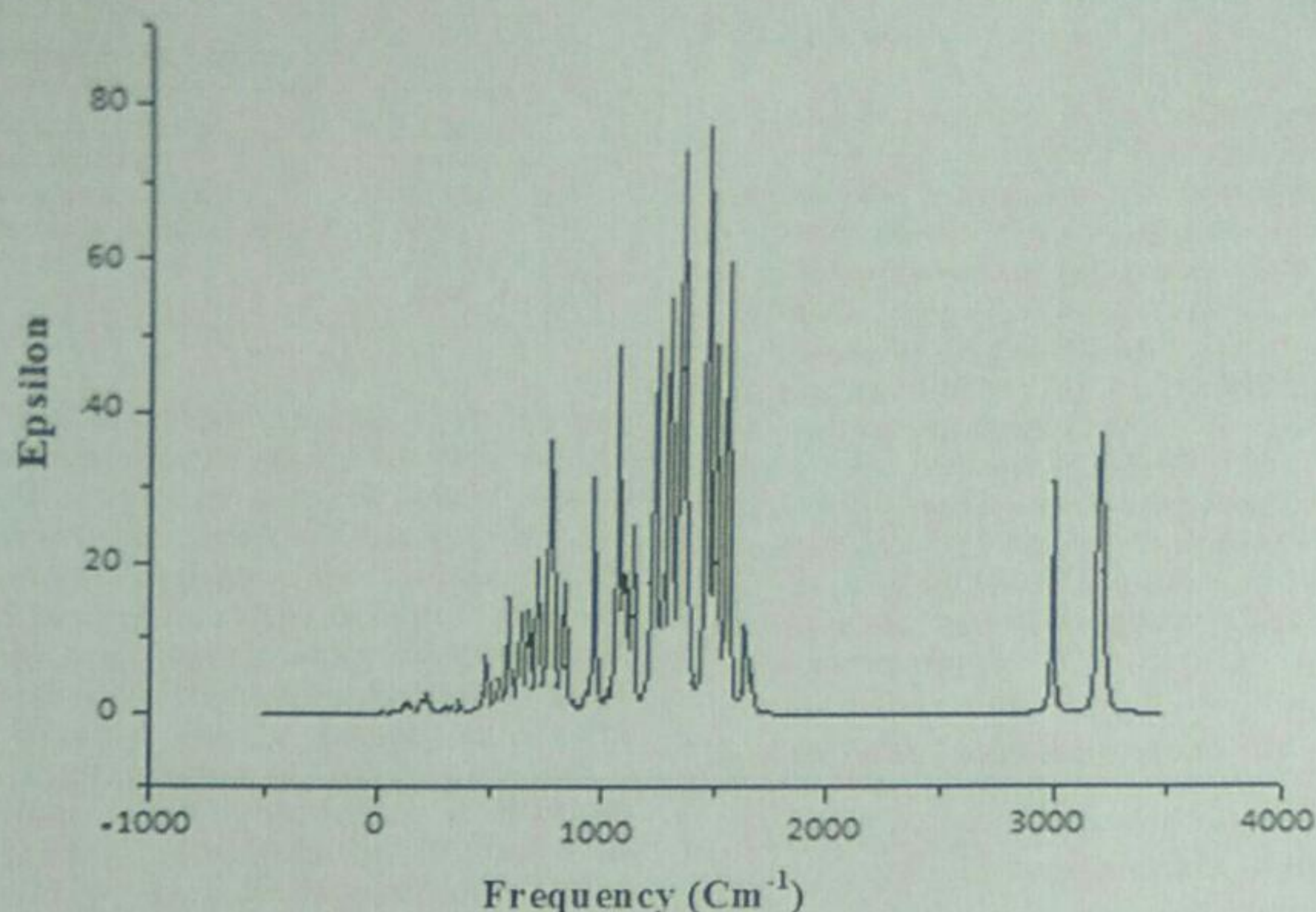


Fig 7. Calculated IR spectra of title molecule by using DFT/B3LYP method.

Table 7

Second-order perturbation theory analysis of the Fock matrix, in the NBO basis for intermolecular interactions within title molecule: Stabilization energy of interactions ($E^{(2)}$), Energy difference between donor (i) and acceptor (j) NBO orbitals ($E_j - E_i$), Fock matrix element between i and j NBO orbitals (F_{ij}).

Donor NBO (i)	Occupancy (i)	Acceptor NBO (j)	Occupancy (j)	$E^{(2)}$ (kcal/mol)	($E_j - E_i$) a.u.	F_{ij} a.u.
π (C1-C2)	0.9897	π^* (C3-C4)	0.1792	10.28	0.28	0.07
π (C1-C2)	0.9897	π^* (C5-C6)	0.1632	10.49	0.28	0.07
σ (C1-C6)	0.9906	σ^* (C1-C2)	0.0070	1.26	1.28	0.05
σ (C1-H7)	0.9914	σ^* (C2-C3)	0.0118	1.88	1.10	0.06
σ (C1-H7)	0.99140	σ^* (C5-C6)	0.0078	1.78	1.10	0.06
π (C3-C4)	0.8334	π^* (C1-C2)	0.1552	10.04	0.29	0.07
π (C3-C4)	0.8334	π^* (C5-C6)	0.1632	9.72	0.28	0.07
π (C3-C4)	0.8334	σ^* (C12-N17)	0.0308	3.11	0.55	0.06
π (C5-C6)	0.8296	π^* (C1-C2)	0.1552	9.60	0.28	0.07
π (C5-C6)	0.8296	π^* (C3-C4)	0.1792	10.54	0.28	0.07
Lp(2) N15	0.9998	π^* (C14-S30)	0.0226	22.72	0.21	0.09
Lp(1) N17	0.9996	π^* (C14-N18)	0.2496	21.09	0.27	0.10
Lp(1) N17	0.9996	σ^* (N18-C14)	0.0337	20.25	0.26	0.09
Lp(2) S30	0.9997	π^* (C14-N18)	0.0138	11.85	0.25	0.07
Lp(2) S30	0.9997	π^* (N18-C30)	0.2145	9.85	0.25	0.06
Lp(3) F29	0.9999	π^* (C22-C25)	0.0135	9.34	0.43	0.09
π^* (N17-C13)	0.1732	π^* (C12-C2)	0.0245	28.45	0.04	0.07
π^* (C22-C25)	0.1840	π^* (C23-C25)	0.0165	153.69	0.01	0.08

properties of molecule. Consequently the compound may be used for NLO materials in future.

3.6. Biological properties

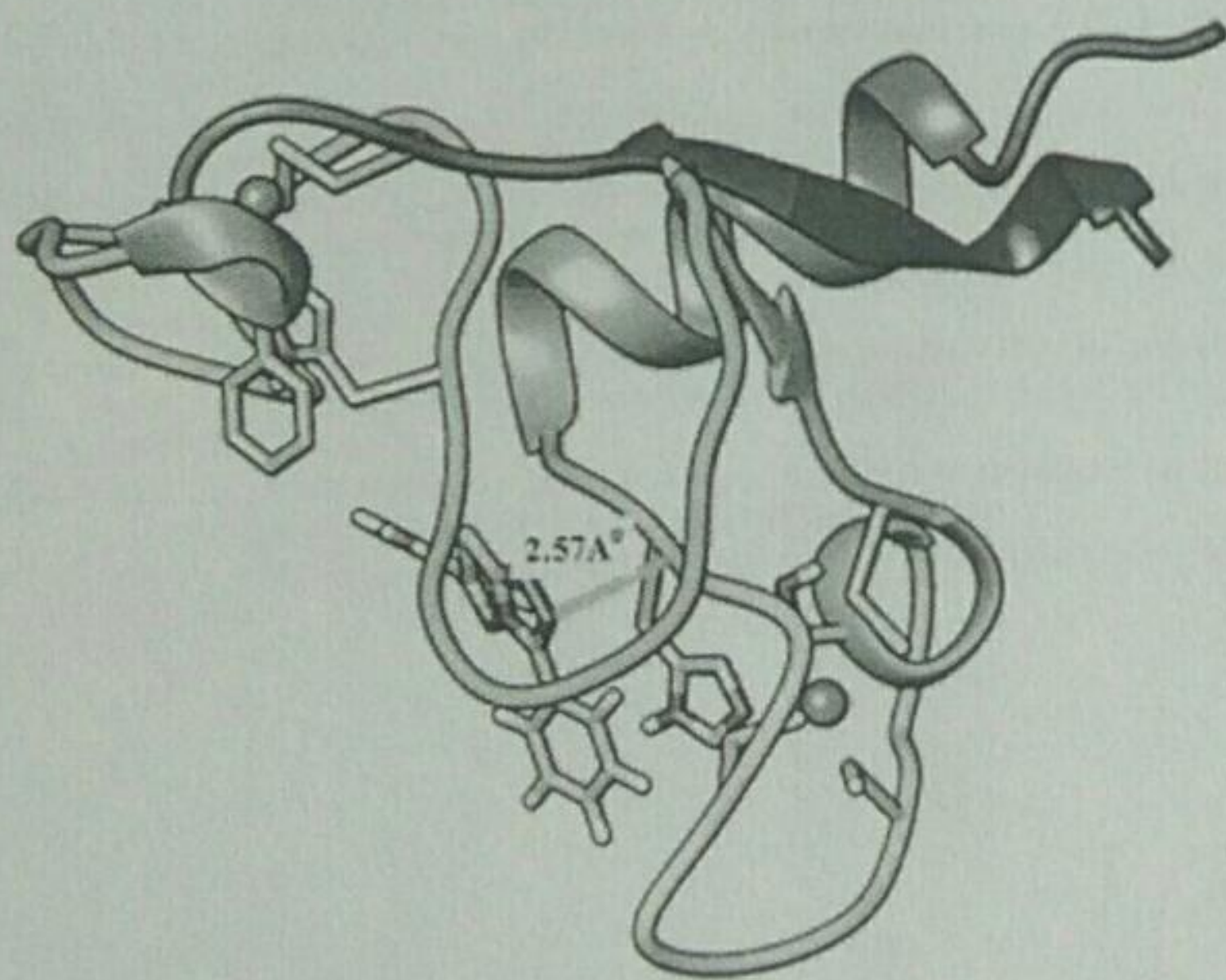
Before discussing the biological activity of the molecule aqueous solubility ($\log S$) and Lipophilicity ($\log P$) are calculated. For evaluating $\log P$ and $\log S$, ALOGPS 2.1 program [63] is used. This program developed by Tetko et al. [64–66] is based on electrotopological state indices and associative neural network modeling. The Structure-property relationship studies are justified by these two parameters. The transport property of drugs and their interaction with receptors are closely related by $\log P$ however bioavailability is closely related by $\log S$. The calculated value of $\log P$ is 2.34 which suggests that molecule is able to diffuse across the cell membranes, so it can be utilized in pharmacological applications. In general 85% of drugs have $\log S$ values in between the range of

–1 to –5.36. The calculated value of $\log S$ (–3.30) further approves the permeability of molecules through cell membranes. Some biological activities of title molecule are calculated with the help of PASS software. PASS calculates 900 pharmacological properties, molecular mechanisms of action, mutagenicity, carcinogenicity, teratogenicity, and embryotoxicity. PASS predicts these properties on the basis of structure activity relationships for the training set, considering more than 46 000 drugs, drug candidates, and prime compounds whose biological activity are resolute experimentally. The calculated results by PASS software have average accuracy of about 85% [67]. In this study we only listed those biological activities, in Table 8, for which $P_a > 70\%$. The molecule shows high value of biological activity for Chloride peroxidase inhibitor. The Chloride peroxidase belongs to the family of enzymes, which catalyzes the chlorination of organic compounds. It employs one cofactor, which may be either heme or vanadium [68]. The molecule inhibits chlorination of organic compounds in blood stream which prevents

Table 8
Some biological activities calculated by PASS with Pa > 70%.

S.N.	Biological activity	Pa	Pi
1.	Chloride peroxidase inhibitor	0.756	0.005
2.	Albendazolemonooxygenase inhibitor	0.688	0.004
3.	Corticosteroid side-chain-isomerase inhibitor	0.682	0.010
4.	Phobic disorders treatment	0.686	0.082
5.	Glucocorticoids	0.646	0.050

bacterial disease. It is used for Phobic disorders treatment also. Phobias are the most common type of anxiety disorder, in which a person experiences an extreme or irrational fear of a place, object, animal, or situation. Corticosteroid side-chain isomers exist in all organs but show highest activity in liver and kidneys. The molecule inhibits Corticosteroid side-chain isomers in liver and kidneys and protect these organ from multiple myeloma. Glucocorticoids (0.646) are part of the response mechanism in the immune system which decreases certain features of immune function, such as drop of inflammation [69]. So they are used as medicines to treat diseases caused by an intense resistant system. They also inhibit growth in cancer cells, therefore high doses of Glucocorticoids are used to treat cancer. This contains inhibitory effects on lymphocyte production, as in the handling of lymphomas and the moderation of side effects of anticancer drugs. Designing new anti-inflammatory in Myotonic dystrophy diseases, agents require the identification of targets, which when inhibited can kill the affected cells. We have done molecular docking studies by using Swiss-Dock web server [70]. MBNL1 receptor is identified as an efficient target, based on the prediction by Swiss-Dock web server. Muscleblind-like (Drosophila), also known as MBNL1, is a protein which is encoded in humans by the MBNL1 gene [71–73]. MBNL1 is stated in the early heart, and its levels rise across fatal and postpartum development. The docking score is expected to have minimum interaction energy value (e-value). As more negative the e-value is the docking becomes more efficient. Docking process does not cover on a specific region but over entire protein. The docking picture of the molecule, obtained from the UCSF chimera software, is shown in Fig. 8. The Full Fitness score for the title molecule is –541.58 a.u. and binding affinity (ΔG in kcal/mol) –5.46 a.u., which suggest that it has good binding affinity. The results obtained from docking studies suggest that the compound can be used as an anti-inflammatory agent in Myotonic dystrophy.

**Fig 8.** Molecular Docking of MBNL1 protein with title molecule.

4. Conclusion

Equilibrium geometries, harmonic frequencies, electronic properties, NBO, NLO analysis, TDDFT and biological activity of title molecule are determined and analyzed using combination of DFT/B3LYP level of theory using 6-311G (d, p) basis set. The theoretical calculation of UV–vis spectra shows a medium intense peak (at 610 nm) corresponding to H-4 → L. The NBO analysis shows that strongest interaction with energy 153.69 kcal/mol corresponding to $\pi^*(C22-C25) \rightarrow \pi^*(C23-C26)$ stabilizes flouro ring. The chemical reactivity of the molecule is explained by energy gap (3.71 eV) and plot of HOMO-LUMO. FF shows that 14C and 31C are better nucleophilic centers however 30S shows better electrophilic center. Full Fitness score corresponding to docking of the molecule with and MBNL1 protein is –541.58 a.u. The molecular docking of title molecule suggests that it can bind and inhibit the receptor enzymes.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ejbas.2018.10.001>.

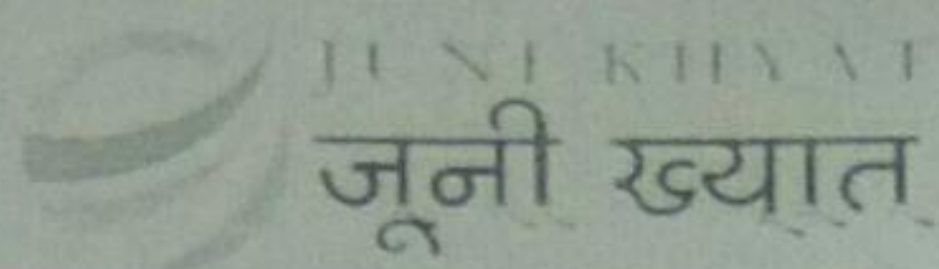
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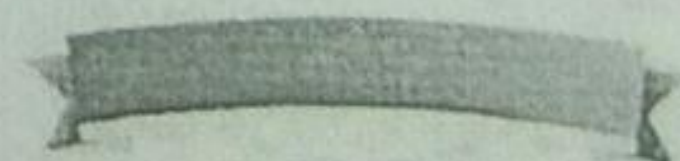


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Kuntal Kishor

**PROBLEMS OF URBAN AMENITIES IN SMALL TOWNS:
A case study of Sitamarhi Municipality**

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Bishrampur, Affiliated to Sant Gahira Gurni University, Surguja, Ambikapur, Chhattisgarh

Abstract:

Urban amenities are facilities, services and infrastructure provided to town dwellers for a better life. Provision and maintenance of urban amenities has been a challenge in small towns of India. Present study is a discourse over the problems of urban amenities in small towns in general and in Sitamarhi town in particular. Author has collected primary data through schedule and interview method during 2016-17 and secondary data from different government and non-government sources. These data have been analyzed with suitable methods and result has been processed at the end. Investigator found many structural and institutional problems in provision and maintenance of urban amenities in the study area. Similar problems have been found by the researcher in other small towns during review of literature. So it can be generalized that small towns in India face problems of urban amenities like poor quality and quantity of infrastructure, services and facilities and lack of civic sense in urbanites together with malfunctioning of institutions involved in provision and maintenance of urban amenities in small towns.

Methodology: present research work is based on the data and information regarding urban amenities in Sitamarhi town. For this study primary data and information has been collected from urbanites residing in Sitamarhi town through schedule and some data and information has been collected through personal interview of ward members and municipal officers. Some information for this study has been collected through empirical observation by researcher. Secondary data has been collected from census report of year 2011. Descriptive analysis of these data and information has been done to get results.

Result: descriptive analysis of data and information collected from the study area reveals that there are several structural and institutional problems of urban amenities in the study area. These problems are mainly associated with provision of urban amenities to the residents and implementation of government programmes for upliftment of the condition of urban amenities in the study area.

Conclusion: Small towns, with lesser fund and without managerial expertise, are not able to provide adequate urban facilities to its inhabitants. On the basis of analysis of data and information gathered from the study it can be said that poor quality of services, inadequate services and facilities, lack of civic sense in urbanites together with malfunction of institutions involved in provision and maintenance of urban amenities are some of the problems found in small towns of India.

INTRODUCTION

Government institutions in India may applaud for their synergy to make one third of Indian population urban but most of the towns, mainly small towns, in India have lesser amenities than rural settlements of United States. Census of India defines a census town as 'a settlement with more than 5000 population having density more than 400 person per square kilometer and where at least 75 % of male working population is engaged in non-agricultural activities'. This definition of town undermines the importance of availability of urban amenities in towns. Poor infrastructure and poor quality of public utility services is characteristic feature of small towns in India. Though some of these towns have more open space and urban green than big towns but

Kuntal Kishor

quality of environment is poor due to impoverished drainage and sanitation facilities in small towns. Lack of public utility services and urban facilities is the only reason behind the fact that 70% of urban population in India live in medium or large towns and only 30% urban population of India lives in small towns of India. Other reasons behind this fact are just consequences of the previous one.

On the basis of population size towns in India can be categorized as; Small Towns having population less than one lakh (1, 00,000), Medium Towns having population one lakh or more but less than one million, Big Town having population more than one million. Out of 7935 towns in India only 465 towns have population one lakh or more. It means more than 94 % towns in India are small towns. About 30% urban population of India lives in these small towns other 70 % urban population is concentrated in 6% towns of India (Census survey, 2011). There is huge gap in population density of medium or large towns and small towns. This difference in concentration of population explains the variation in provision of urban amenities in small towns and big towns. Not only the size of population is low in small towns of India but the facilities, services and infrastructure are also poor here. Dr. Kuntal Kishor (2018) found that although most of the resident population in Sitamarhi town, a small town in Bihar province of India, is satisfied with the services and facilities they get but condition of these services and facilities is very poor and need to be improved as soon as possible.

Small town as a center of economic development

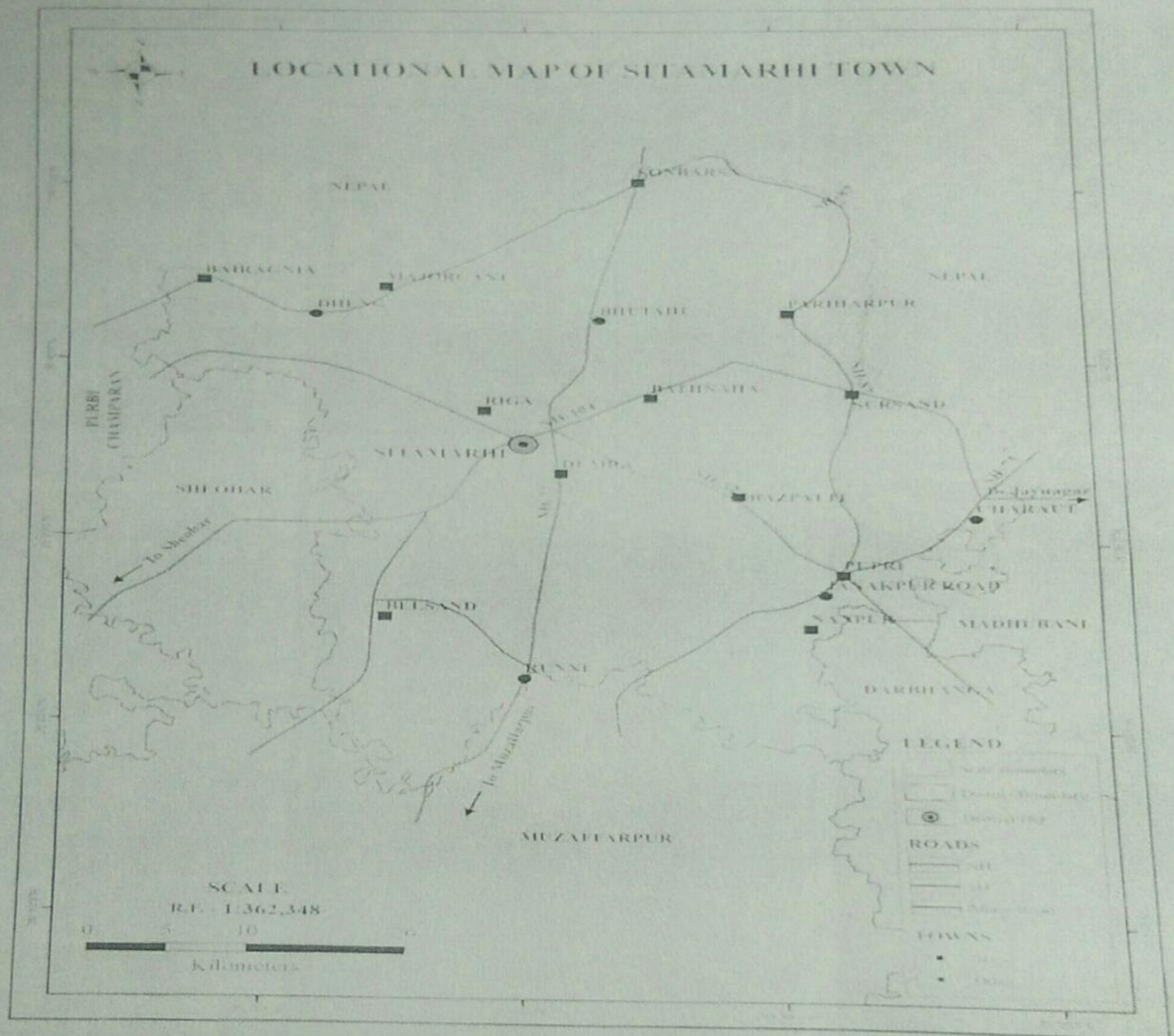
Small towns play important role in development of country in general and rural hinterland in particular. The symbiotic relationship between rural and urban settlement is clearly visible in around small towns (Cecilia Tacoli, 2017). Small town provide non-agricultural employment to rural population and add value to the agro products from rural areas through small food processing units in these small towns. For local small farmers these towns are affordable market and service centers. Small town receives raw material for food processing units and cheap laborer from rural hinterland. These small towns also provide educational, medical and recreational facilities to rural hinterland. Like other towns Sitamarhi town provide employment to rural hinterland. For the same hinterland Sitamarhi town is service center and market. The area of influence of Sitamarhi town, on the basis of method adopted by V.L.S. Prakash Rao, is a circular 65 km^2 area having radius of about 4.5 kilometers

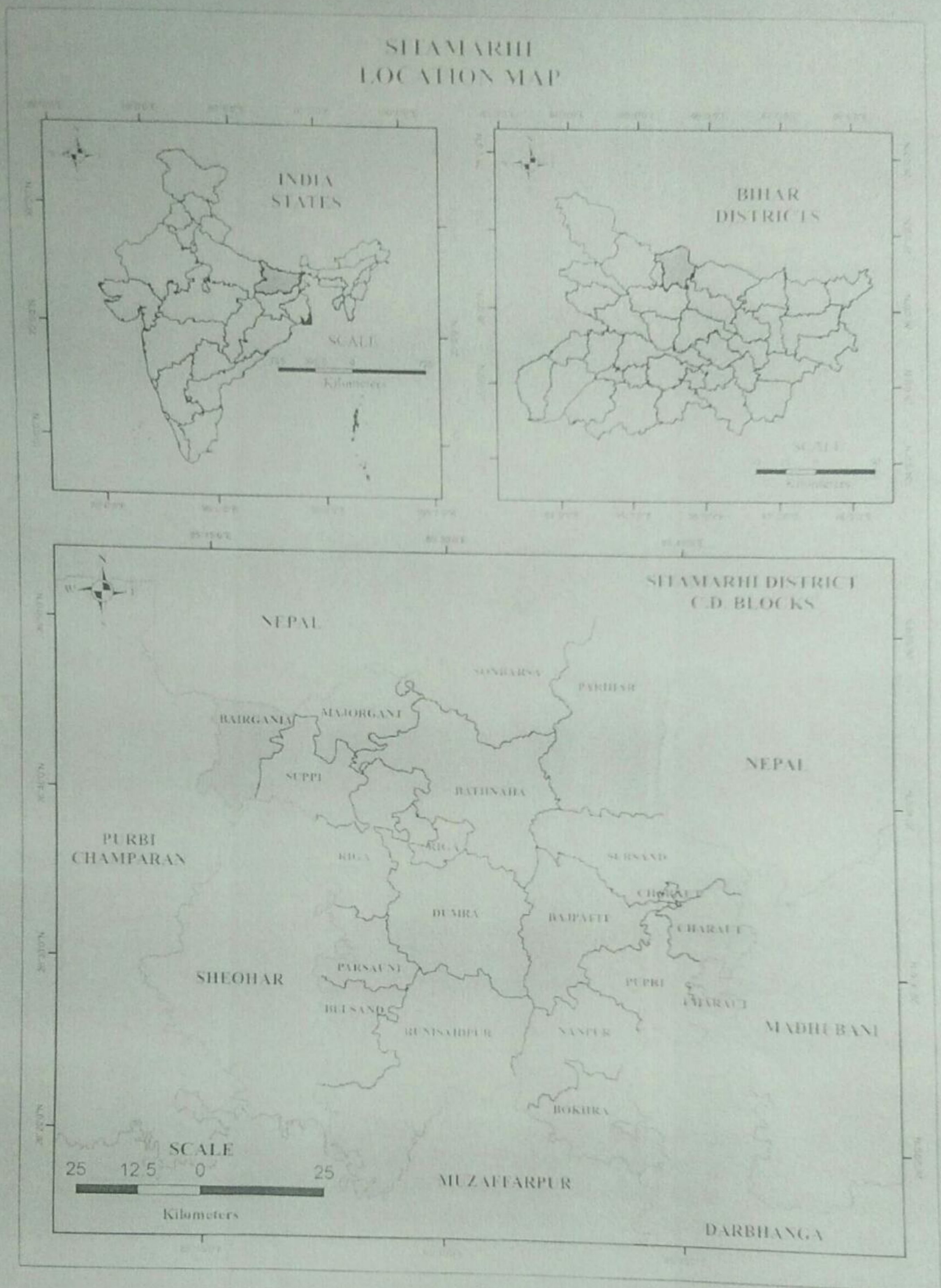
Small town as a safety valve for big cities

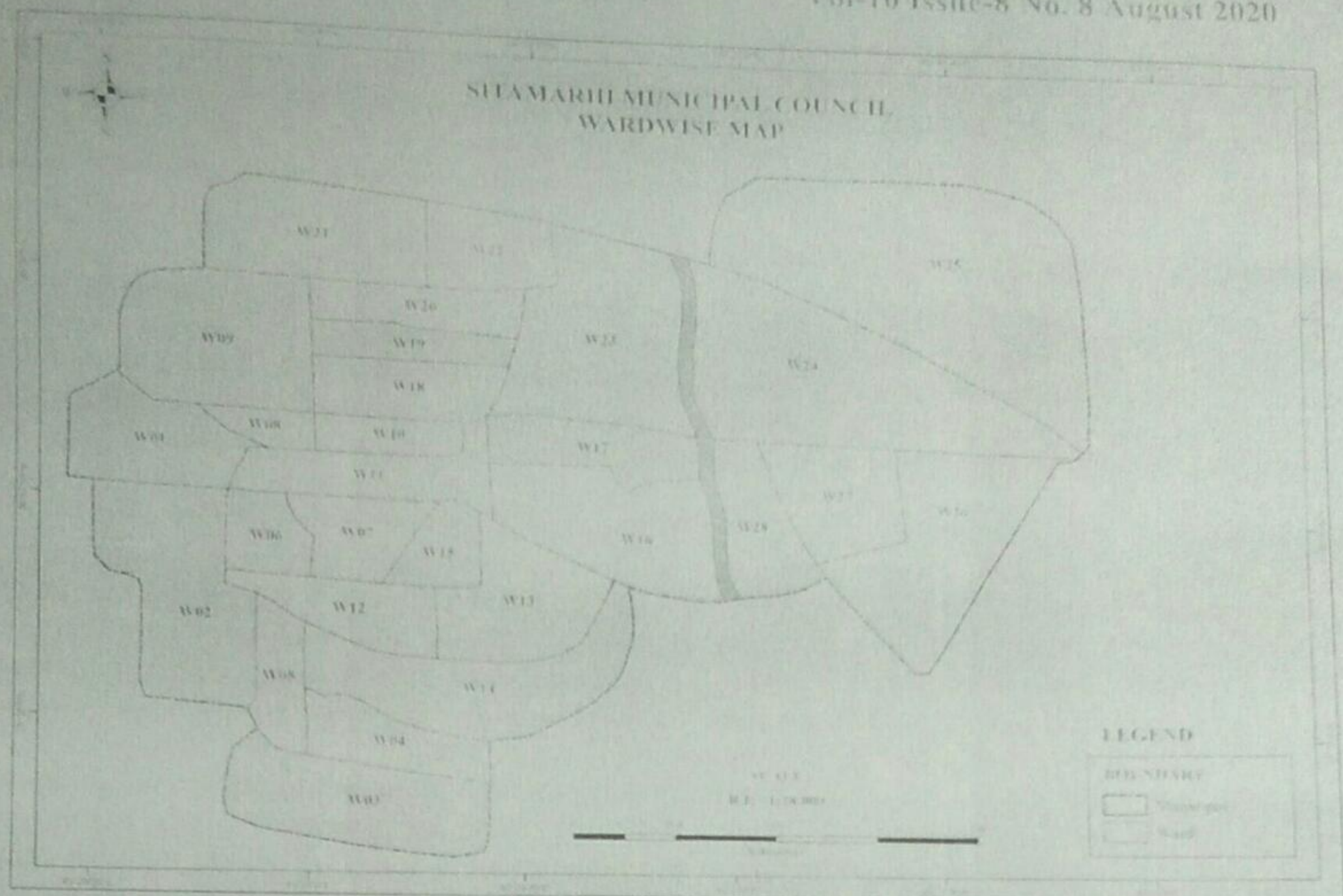
Small towns reduce pressure of population in big cities in India. It can be further improved by development of small towns. The resource and population ratio is decreasing day by day in big cities of India due to large scale flow of immigrants from small towns and rural areas. Further, high density of population, traffic congestion, slum development, increase in crime rate and many other problems are related with huge rate of immigration in big towns. Increase in population of big towns of India adds to the burden of local governing bodies for provision of services and facilities in limited resources. As a consequence quality of public utility services and urban facilities have deteriorated in these towns. Development of small towns could attract more immigrants from rural area and check emigration from small towns and condition in big cities could also improve in this way. So these small towns are safety valve for big cities from where big city can release pressure of population. Small towns can be improved to a center of excellence in provision of services, employment and education through investment in secondary and tertiary sectors.

STUDY AREA

The study area of present research work is Sitamarhi town which is the district headquarter of Sitamarhi district of Bihar.







Sitamarhi district is situated in northern part of middle Ganga plain of Bihar. The town Sitamarhi is administrative unit (Municipal Council) of Dumra block and situated in the center of the block. National Highway 77 connects it to Muzaffarpur and Patna district to the South. State highways link it to Madhubani district in the east and Sheohar district in the west. The town Sitamarhi is situated on the Darbhanga-Narkatiaganj railway line and has the largest railway station of the district. There is another broad gauge track, running between Muzaffarpur and Sitamarhi. Sitamarhi municipality was constructed in 1882 with a municipal board consisting of 12 commissioners. At that time there were only 4 wards in the town. (**Bihar District Gazetteers Muzaffarpur, 1958**) Now the municipality is divided into 28 wards. Dumra Notified Town Area Committee was constituted in 1937. Sitamarhi urban agglomeration occupies Dumra Notified Town Area as a statutory town. At present most of the government offices of Sitamarhi district are situated in Dumra. Sitamarhi is located in Mithila cultural region which is a part of Tirhut Division of Bihar.

The study area, Sitamarhi municipal council is situated almost in the center of Sitamarhi district, within Dumra block and occupies an area of about 5 square kilometer. The shape of Sitamarhi municipal council (SMC) is almost rectangular. The SMC has maximum east-west extension of 4.5 km and maximum north-south extension of 3 km. The site of the town Sitamarhi is a flood free site on natural levee of river Lakhandei. The municipal council has rivarian situation on both side of the river Lakhandei and has an important location at the confluence of state highway and NH 77, and along Darbhanga-Narkatiaganj railway line.

OBJECTIVE

This study is aimed to find out the problems associated with provision and maintenance of urban amenities in small towns in general and in Sitamarhi town in particular. The study also tries to find out the reason behind different problems of urban amenities. Specific problems of urban amenities in small towns are also within the scope of this study.

METHODOLOGY

This study is based on primary data and information collected from urbanites residing in Sitamarhi town through schedule and data and information collected through personal interview of ward members and municipal officers. Some information for this study has been collected through empirical observation by researcher. Secondary data for this study has been collected from different government and non-government journals, periodicals and census survey reports. These data have been analyzed with suitable methods to process information regarding problems of urban amenities.

URBAN AMENITIES

Urban amenities are goods, services and facilities that people appreciate about their environment. These are services and facilities that make any town livable and comfortable. Urban amenities can be considered as public goods and services for collective consumption (Castells, 1977). Urban amenities means the facilities provided to urban population for a good, comfortable and healthy life (Kuntal Kishor, 2018). Michael Pacione (2009) has identified three basic characteristics of urban amenities; joint supply, non-excludability and non-rejectibility. Condition of urban amenities predicts the future growth of the town. Better amenities always attract population and investment. So, urban amenities are essential pre-requisite for socio-economic and physical growth of town. The provision of urban amenities in towns is one of the most important functions of welfare government. These are also essential for revenue generation. Equal and just distribution of urban facilities and services is a challenge for local governing bodies in towns of developing countries like India.

PROBLEMS OF URBAN AMENITIES IN SMALL TOWNS (SITAMARHI)

Equal and just distribution of urban amenities and maintenance of its quality and quantity according to the need of urbanites is the main aim of government agencies and Urban Local Bodies (ULBs). The difference in demand and supply of urban amenities is due to several problems related with provision and maintenance of urban amenities. Small towns with small fund, low managerial and technical know-how of ULBs, unskilled workers face different problems than big towns where governing bodies and workers are skilled and trained and funds from public and private (or both) agencies received regularly. More or less, all small towns face similar problems of urban amenities. The problems of urban amenities in small towns (especially Sitamarhi town) have been categorized by Kuntal Kishor (2018) in two classes; Structural problems and Institutional problems.

(i)	Structural Problems	Inadequacy of services and facilities
		Poor quality of services and facilities
		Lack of civic sense in Urbanites
(ii)	Institutional Problems	Spatial and social variation in distribution of services.
		Poor maintenance of services and facilities
		Improper implementation of programme.
		Overlap of the area of services with

Kuntal Kishor

Source: Unpublished PhD Thesis of Kuntal Kishor, Patna University, 2018.

(i) **STRUCTURAL PROBLEMS:**

Structural problems are associated with the basic social and cultural structure of the town, characteristics of population and available infrastructure.

Inadequacy of services and facilities

The problem of inadequate services and facilities is due to lack of fund for development of necessary infrastructure. Most of the small towns in India face this problem and Sitamarhi town is not an exception. Problem of inadequate facilities and services in the town has been mentioned below.

1. Lack of number of workers in municipal council for sanitation work.
2. Inadequate fund for development of drainage and sewage.
3. Inadequate power for continuous supply of electricity.
4. Inadequate number of dustbins for storage of domestic waste.
5. Inadequate number of street lights.
6. Inadequate number of shopping mall and parking places.
7. Absence of sewage treatment plant.
8. Insufficient number of multi-speciality hospitals.
9. Insufficient infrastructure for industrial development.
10. Absence of footpath for pedestrian.
11. Absence of technical (Medical/Engineering) colleges in the town.
12. Inadequate infrastructure for water supply to slum dwellers.

Similar problems of inadequate urban amenities have been found in different small towns e.g. Bettiah (Md. Hussain Ansari, 1991) and Saharsa (Anant Bhagat, 2016).

Poor quality of services

The town Sitamarhi is one of the poor cities in Bihar in terms of quality of services provided here. The municipality and parastatal agencies of Bihar government (like PHED, Bihar Electricity Board, BSNL, DEO office and Banks etc) are responsible to provide physical, social and financial public amenities to the urban residents. These agencies are unable to provide the good quality services partially due to lack of fund and resources and partially due to lack of determination of the agencies to provide basic civic services to the residents and properly implement the plans and schemes regarding provision of basic urban amenities. Lack of managerial and technical knowhow in local bodies is also responsible for poor quality of services. Main problem of urban amenities in terms of its quality are following:

1. Lack of wide good quality roads.
2. Lack of facilities for pedestrian and street vendors (separate space on roads).
3. Lack of good quality institute for higher education.
4. Poor quality of drainage system in few pockets of slums of Sitamarhi.
5. Poor quality of community toilets.
6. Poor overall environmental condition and lack of beauty of urban landscape.

Kuntal Kishor

7. Lack of good quality intensive and emergency care medical facility, for which town dwellers depend on SKMCH (Muzaffarpur) and PMCH (Patna) and others Hospitals outside the town.
8. Poor quality of sanitation services.
9. Poor quality of urban solid waste disposal (disposal without treatment along the Ring Road).
10. Poor quality of bus Depot (stand) and vehicles parking places.
11. Dustbins placed to collect Household solid wastes are too small to accommodate the domestic wastes of all household of the colony.

Poor quality of public utility services is a common problem in small towns of India. Aforesaid problems were also observed by O. P. Prasad in Buxar (2005) and Md. Hussain Ansari in Bettiah (1991).

Lack of civic sense in Urbanites

Alexander Badawy (1967) in his article "The civic sense of Pharaoh and urban development in ancient Egypt" put emphasis on importance of civic sense in urban residents in development and maintenance of any urban landscape. Lack of civic sense in residents of Sitamarhi town is expressed through their following behavior:

1. Many of the town dwellers throw solid waste in drain.
2. Urbanites in the town litter garbage on roads.
3. Sometime they do not follow traffic rules.
4. Town dwellers do not keep public property clean and sometime destroy it.
5. Many of the residents of town have illegal electricity connection to elude the electricity charges.

(ii) INSTITUTIONAL PROBLEMS:

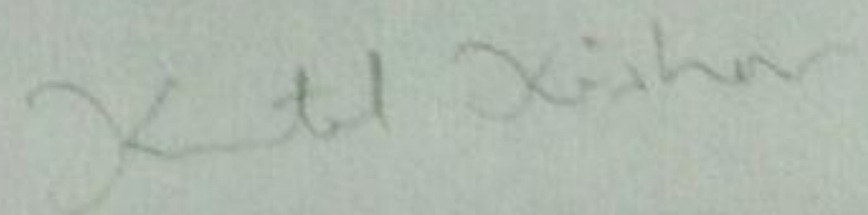
Institutional problems of urban amenities are due to discrepancy in involved government institutions. More or less all small towns in India face similar institutional problems in provision and maintenance of urban amenities. Some of these problems found in Sitamarhi town have been discussed below.

Spatial and social variation in distribution of services

Intra-ward variations in distribution of services and facilities in study area are mainly due to the reason that the areas inhabited by influential person are better served than the other areas of ward. Inter-ward/Inter-colonial variation in distribution of facilities is mainly the result of ecological process of evolution of the town. During evolution of Sitamarhi town socially and economically backward class (laborer of unorganized sectors) settled in the area of low rental value. These areas became slum during gradual development of the town and these are the least served areas having lowest sanitation, drainage and toilet facility and temporary (kacheha) houses. So, inter-ward variation is result of social segregation processes. Almost all small towns in India face problem of unequal distribution of urban amenities like Sitamarhi town.

Poor maintenance of services and facilities

Urban amenities need to be regularly maintained for their long life and proper functioning. Maintenance of urban infrastructure, services and facilities is function of government agencies in Indian towns. In Sitamarhi town, like other



small towns in India, regular maintenance of urban amenities is not performed due to following reasons:

1. Unwillingness of government agencies.
2. Lack of fund for renovation and maintenance of urban amenities.
3. Absence of public support for renovation activities.
4. Misuse of public properties by town dwellers.

Improper implementation of programme

Importance of small town is well recognized by the governments in India. There are many programmes launched by states and central government for development of small towns. Implementation of these programmes is task of executive bodies. But proper implementation of programmes related with development of urban amenities in small towns is not done due to:

1. Lack of technical and managerial knowhow in governing bodies.
2. Lack of determination for implementation of programmes.
3. Conflict between parastatal agencies.
4. Lack of fund for proper implementation of programmes.
5. Corruption and local politics.

Similar problems of improper implementation of programmes have been found by different scholars in different small towns of India.

Overlap of the area of services with parastatal agencies

"In all the cities, service delivery is fragmented, with multiple entities involved in each service. These entities are also often accountable to different departments of the state government, which means that reform also has to involve state governments. Fragmentation of responsibility of service delivery and its duplication are common phenomena." (David Savage and Shubhagato Dasgupta). Duplication of responsibilities creates confusion in government agencies and so provision of amenities to town dwellers is not done properly. Sometimes different agencies blame other agencies for irregular and poor quality of services and no agency take responsibility of the misdeeds. 'In Sitamarhi town supply of water is responsibility of both Municipality and Physical Health and Education Department (PHED). The duplication of functions of government bodies always lead to confusion in implementation of schemes. The clear division of function between different agencies of government is necessary for proper functioning of different bodies and better implementation of programmes and schemes' (Kuntal Kishor, 2018).

CONCLUSION

Urban amenities are the facilities, services and infrastructure that people in town want to have for better life. Provision and maintenance of urban amenities in small towns of India has been a challenge for local governing bodies. The problems of urban amenities in small towns of India are different from the problems in big towns. Poor quality of services, inadequate services and facilities, lack of civic sense in urbanites together with malfunction of institutions involved in provision and maintenance of urban amenities are some of the problems universally found in small towns of India.

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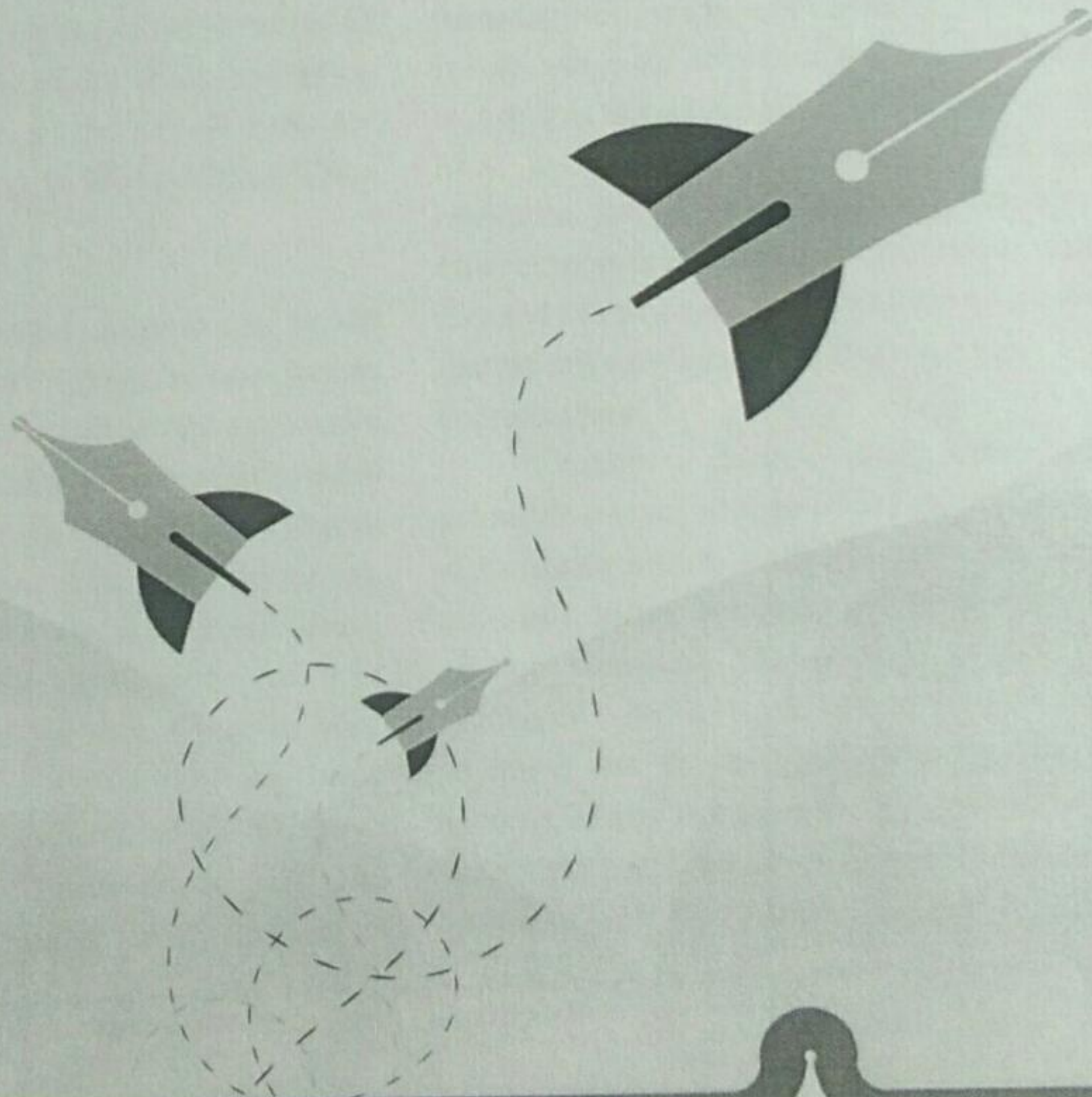
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CREATIVE COMPONENTS MAKES CREATIVE ADVERTISING : AN ANALYSIS

□ Dr. Pradeep Kumar Srivastava*

ABSTRACT

Creative components are means for helping creative people to final new and relevant ideas to carry their themes in advertising. Creative advertising has now become an indispensable activity in our economy and its significance is increasing year after year. Its need has arisen due to the sweeping changes in the life of everyone. Actually after economic liberalization Indian advertising industry witnessed a boom. The entry of many MNCs in India has further added new variety of feathers to the growth-cap of advertising. Advertising expenditure in India has been increasing rapidly. It is only because of creative advertising is considered one of the most vital areas of investment. The objective of the present study is to examine the different creative associations which make the advertisement creative.

Keywords : Creativity, Innovation, USP, Relevance, Execution, Incubation , Illumination

Methodology

The research work has been undertaken to explore requirements, impact and the analysis of creative association in advertising. This is descriptive in nature. In order to achieve the objectives of the study secondary sources of data have been used viz., Centre for Monitoring on Indian Economy (CMIE); FICCI- Price waterhouseCoopers report.

Result

There are different creative components which make advertising creative like creative association, creative idea, creative process etc. A number of creative associations that may be in the advertisement like Unique Selling Proposition, relevance, jingle, slogan, positioning, celebrity, execution, humor, branding etc. which makes advertisement creative. Preparation, incubation, illumination, and verification are four established stages of creative process. Creative idea, creative process and creative association are basic components of creative advertisement. Creative advertisement is now become necessary to exist and make competitive in the market with maximum

profitability.

Conclusion

Creative advertising has now become an essential parameter to every type of advertisement in our economy. it will create the relevance of creative components that are capable to make an advertisement creative. The one of basic components are creative association like usp, relevance, jingle, slogan, branding, celebrity humor etc other components are creative ideas and creative process. Its need has emerged because of the major developments that are influencing the life of everybody.

Introduction

Economic reforms attempted as of late have achieved a great change in the economic environment. Advertising sector, alongside different segments of the economy, has additionally profited by and large by the change measures. The passage of MNCs, in India, combined with the battle of customary Indian corporate to make due in the market brought about expanded volume of ads from contending brands. Indeed, Indian advertising industry saw a genuine 'commercial boom' in post economic liberalization time. The section of MNCs

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in India has additionally added new plumes to the development top of advertising. Satellite TV stations have strengthened its development example and structure. The utilization of cutting edge devices and methods has incredibly improved its quality and execution. Promoting of budgetary administrations has injected new force and eagerness into advertising.

Creative Components in Advertising

Creative components are means for helping creative people to final new and relevant ideas to carry their themes in advertising. While creative advertising is referred to as an art which is original, relevant, noticeable, memorable and refreshing in its presentation. A creative packed advertisement should be pure, simple and honest in its presentation. The use of association is the most common creative problem solving techniques inexistence and the making of association is basic to the creative mind. Thus, associations are means for helping creative people to final new and relevant ideas to carry their themes.

The need for creative advertising is quiet from the fact that there are uncountable ads and commercials bombarding our daily lives, yet only a few of them are remembered as creative. The reasons for advertisements not being read as a self oriented approach rather than as market oriented approach and lack of creative approach. A creative advertisement, whether in terms of ideas or execution or both, will stand out, provoke interest, and bring prestige and attention. There is pure creativity, as in fine art, there is applied creativity. Thus advertising creativity is a sort of applied creativity. Creativity is simply a technique for producing ideas to achieve something new and relevant. Webster² defines creativity as "the ability to bring something new in to existence". It is the most important aspect of the advertising effort because it determines success or failure for a marketer. Advertising with creative ideas requires a human touch and theme. Newness and relevance are the basic characteristics of creative ideas. To be more specific and relevant, each advertising agencies go with new creative ideas to ensure their prosperous marketing. Creativity in advertising is defined, by Hepner (1956)¹, as having two characteristics: first, the originality evident in the

message communicated and in its presentation, and second, the improvement made in the life of consumers or effect on the consumer's standards of living.

The requirement for creative advertising hushes up from the way that there are uncountable promotions, advertisement and plugs assaulting our everyday lives, yet just a couple of them are recognized as imaginative. The explanations behind notices not being perused as a self situated methodology as opposed to as market arranged methodology and absence of innovative methodology. An innovative commercial, regardless of whether as far as thoughts or execution or both, will stick out, incite intrigue, and bring glory and consideration. There is unadulterated innovativeness, as in compelling artwork, there is applied imagination. In this way publicizing imagination is such an applied inventiveness. Imagination is essentially a procedure for creating thoughts to accomplish something new and important. Webster² characterizes creativity as "the capacity to bring something new in to presence". It is the most significant part of the promoting exertion since it decides achievement or disappointment for an advertiser. Promoting with inventive thoughts requires a human touch and subject. Originality and pertinence are the essential attributes of innovative thoughts. To be more explicit and applicable, each publicizing offices go with new inventive plans to guarantee their prosperous promoting. Inventiveness in publicizing is characterized, by Hepner (1956)¹, as having two qualities: first, the creativity apparent in the message conveyed and in its introduction, and second, the improvement made in the life of purchasers or impact on the customer's ways of life.

There are different creative components which make advertising creative like creative association, creative idea, creative process etc. A number of creative associations that may be in the advertisement like Unique Selling Proposition, relevance, jingle, slogan, positioning, celebrity, execution, humor, branding etc. which makes advertisement creative.

Objective of the Study

The objectives of the present study are :

1. To explore the creative association in

advertisement

2. To highlight the determinants of creative advertising

Literature Review

Elms (1995)³ has given two major components of creative strategy are first is message content and second is message execution.

Jewler and Drewniany (2001)⁴ say that an ad "needs to contain a persuasive message that convinces people to take action". To be more creative, however, they suggest that an ad "must make a relevant connection with its audience and present a selling idea in an unexpected way.

William et. al. (2004)⁵ says that effective ads work on two levels. First, they should satisfy consumer's objectives by engaging them and second, delivering a relevant message.

Creative Ideas

An idea must be novel and relevant to be creative. Both the qualities are as two wheels of two wheeler motor cycle. If one of them is not present in any idea, that will not be creative. Creative ideas are novel and relevant realities resulting from connection of old realities. Often this is by-product of analogical or metaphorical thinking.

Creative advertising ideas require some basic norms such as adaptability, durability, newness, oneness relevance, memorability and simplicity. This 'ADNORMS' are characteristic standard of quality found in the most creative advertising ideas. Off-course, we could not ensure that all creative advertising ideas will satisfy or possess the entire above characteristic to meet standards of quality but they are considered as goal for the creative advertising mind. Marra (1990)⁶ pointed out that creative advertising ideas were uniquely and strategically positioned in the target audience's mind. Their newness and rightness ensure their productivity which are durable and satisfier of market requirement. With above ADNORMS we can examine creativity in advertising ideas.

Creative Process

Joseph Wallas, who proposed that creative thinking proceeds through four phase: stage of creative process: preparation, incubation, illumination, and

verification. Preparation is the phase during which the creative person does all the preliminary work. He thinks in a sort of free way, he collects he searches, listens to suggestions, and lets his mind wander. The stage of incubation is inferred from the fact that a certain period of time, ranging from a few minutes to months or years, elapses between the period of preparation and that of illumination⁷. This period may be variable length as the person turns to his everyday business. The third stage illumination presents the emergence of an idea or a solution to a problem. The creative individual after analyzing existing ideas and verifying the old one submit a solution to the best of his ability in respect of problem selected under creative process. The last stage of verification, at this stage actual working of the idea take shape and the creative individual find out the creative ideas as a final solution after verification. On the other hand Taylor retains Walla's four stages but also believes that creativity exists at five different levels..

Every models of the creative process are base on the steps in the creative process. The creative process is going through the stages of orientation, preparation, analysis, ideation, incubation, synthesis and verification. Thus, we can say that the primary objective of creative process is a person, a problem and a solution.

Approach towards Advertising

In India the main Advertising Convention was set up in Kolkata in 1960's. As per Dr. Keskar, The promoting ought to be Indian in thought and substance. In 1980, there was an extension in both electronic and print media. The idea of supported software engineers on TV was start presented for "Murmur Log" famous drama in 1983, at that point came "Buniyaad, Nukkad" and "Mahabharata" and "Ramayana" from 1986 ahead which was appeared in Doordarhan with no serious channels. 1990s was the year for satellite stations, which assisted the promoting scene with thriving completely fledged.

Subsequent to picking up Independence the matter of publicizing slowly began cutting a reasonable specialty in social and monetary arrangement of the nation. Notwithstanding, till 1970s Indian business sectors had restricted presentation to rivalry. Markets were practically vender arranged. In an economically

tight market, the dealer needs advertising with the sole reason for anticipating a picture of the venture in the brains of clients. The whole publicizing program is intended to suit the customer's likes instead of definitive clients. Consequently, promoting involves a little specialty in the whole range of showcasing procedure of the seller¹.

During this time, creative advertising becomes essential prerequisite to address the difficulty for advertising of a specific item. The customer is lord in free undertaking framework and his needs will decide handiness of items. In light of the current situation private associations as well as open endeavors will undoubtedly focus on the part of creative advertising to get the considerations of focused shoppers, and to get the most extreme consideration, they are offering items and administrations upheld by creative advertising. Thus, Creative advertising has become an imperative movement in our economy and its noteworthiness is expanding a seemingly endless amount of time after year. Its need has emerged because of the far reaching developments that are influencing the life of everybody. Creative advertising is presently an acknowledged force in the business world. Anyplace we go, we notice a plenty of notices around us, disclosing to us various messages. Inventive promoting gives the open the option to pick between numerous choices, numerous brands. It empowers shoppers to pick the best quality or the most minimal cost or the best blend of value and cost. The financial specialists everywhere on over the world have discovered that it is a powerful and productive investment.

Findings

Creative advertising has been characterized and examined by the different researchers with various method of examination in a given point of view. Various models have additionally been proposed to pass judgment on the imagination face to face, thought, ads and showcasing. Defenders of creative advertising have consistently concurred that creativity was essential prerequisite to sell or to set up each item in the serious market and it is result of creative components that will make the advertisement creative. Discussions and

theories have been created to explain method of creativity and its significance. The accompanying segment presents the primary discoveries of the examination:

- Creative advertisement is now become necessary to exist and make competitive in the market with maximum profitability.
- Creative idea, creative process and creative association are basic components of creative advertisement.
- Creativity and innovation are two basic pillars of an advertisement for productivity and sustainability.
- Originality and imagination are useful in creativity and also expected to make feasible solution to real problems, despite profitability.
- Preparation, incubation, illumination, and verification are four established stages of creative process.
- Creative ideas are very dependent on these qualities of newness and relevance. Such creative ideas relating to advertisement possessed adaptability, durability, oneness, newness, relevance, memorability, and simplicity. Therefore, creative advertising ideas are uniquely and strategically positioned in the target audience mind.

Conclusion

During the current period, imagination in promoting becomes essential prerequisite to address the difficulty for advertising of a specific item. The buyer is ruler in free endeavor framework and his needs will decide value of items.

Thus, creative advertising has now become an essential parameter to every type of advertisement in our economy. it will create the relevance of creative components that are capable to make an advertisement creative. The one of basic components are creative association like usp, relevance, jingle, slogan, branding, celebrity humor etc other components are creative ideas and creative process. Its need has emerged because of the major developments that are influencing the life of everybody. Planning, brooding, light and confirmation stages were important to produce inventive thoughts

along with this imaginative people must work in durable group to use their likely capacities.

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Research Today

रिसर्च टूड

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सिन्धु घाटी सभ्यता का भौगोलिक परिचय

डॉ० कुन्तल किशोर,

सहा० प्राध्यापक (भूगोल)

शासकीय महाविद्यालय बिश्रामपुर संत गहिरा गुरू विश्वविद्यालय

आम्बिकापुर, छ० ग०

डॉ० कुमार पुरूषोत्तम सुमन

शोधार्थी भूगोल विभाग, पटना विश्वविद्यालय, पटना

सारांश

मानव इतिहास में कई सभ्यताओं का उदय एवं अस्त होता रहा। इन सभ्यताओं का विकास निश्चित रूप से स्थानीय भौगोलिक परिदृश्य की अनुकूलता के कारण हुआ और इन सभ्यताओं का विनाश भी भौगोलिक एवं भूराज्यिक परिस्थितियों में बदलाव के कारण हुआ। सिन्धु घाटी सभ्यता विकास 5000 ईसा पूर्व से भी पहले भारतीय उपमहादीप के उत्तरी-पश्चिमी भाग में हुआ। इस प्रदेश की भौगोलिक परिस्थिति कृषि एवं मनुष्यों के विकास के अनुकूल थी। इस सभ्यता की आर्थिक सामाजिक परिस्थितियों का अवलोकन करने पर पता चलता है कि यह सभ्यता अपने समय की सर्वाधिक विकसित सभ्यता थी जहाँ आर्थिक एवं सामाजिक उन्नति के लिए व्याप्त अधोसंरचना विकसित हुई थी। शहरी क्षेत्र का ground plan/ layout का अध्ययन करने से यह पता चलता है कि शहरी अधोसंरचना का विकास सुनियोजित तरीके से हुआ, जहाँ सभी निवासियों के लिए सभी शहरी सुख-सुविधाओं मुहैया कराया गया था। इस सभ्यता की स्थिति (Site) एवं अवस्थिति (Situation) एक ऐसे भूभाग पर था जहाँ अनुकूल जलवायु मिट्टी, पानी एवं जल अथवा स्थल यातायात की सुविधा उपलब्ध थी।

अपने विकास के चरम पर यह सभ्यता एक आदर्श शहरी सभ्यता के रूप में विकसित हुआ। कालांतर में भौगोलिक परिस्थितियों के बदलाव मुख्यतः जलवायु परिवर्तन एवं नदियों के सुखने के कारण धीरे-धीरे इस सभ्यता ने अपना पूर्व स्वरूप खो दिया तथा ज्यादातर निवासी अन्यत्र अनुकूल भौगोलिक प्रदेश में चले गए इस तरह इस सभ्यता का अंत हो गया।

सिन्धु घाटी सभ्यता का भौगोलिक परिचय

परिचय

सिन्धु घाटी सभ्यता के विकास का प्रारंभ लगभग 7000 ई. सा. पूर्व में बलुचिस्तान के मेहरगढ़ से हुआ। प्रारंभ में यहाँ के लोग कृषक थे। सिन्धु एवं उसकी सहायक नदियों ने इस सभ्यता को पाल-पोस कर बड़ा किया। जनसंख्या बढ़ने एवं नए कृषि योग्य भूमि की खोज के कारण इस मानव बसाव के क्षेत्र में विस्तार होता गया। कृषि उपज की अधिकता एवं संपन्नता के कारण नई जरूरत के अनुसार नए व्यवसायों मुख्यतः व्यापार कारीगर इत्यादि का भी विकास हुआ। कालान्तर में 2600 ई० पू० से लेकर 1800 ई० पू० के बीच यहाँ शहरों का विकास हुआ संभवतः इस सभ्यता में सर्वप्रथम व्यावसायिक विशेषज्ञता का उद्भव हुआ। सभी समुदाय चाहे वह कृषक हो व्यापारी हो कारीगर हो या फिर पदाधिकारी हो सभी ने अपने काम में निपुणता हासिल की क्योंकि बिना व्यावसायिक विशेषज्ञता के इस तरह के सभ्यता का विकास होना संभव नहीं था। कई इतिहासकारों ने सिन्धु घाटी सभ्यता का समय 5000

Kuntal Kishor

ई0पू0 से 1500 ई0पू0 निर्धारित किया है लेकिन अलग-अलग प्रमाणों से यह प्रकट होता है कि सभ्यता का विकास कई सैकड़ों में हुआ। एवं 5000 ई0पू0 से 1500 ई0पू0 तक यह सभ्यता पूर्ण रूप से विकसित थी। अपने विकसित स्वरूप में यह सभ्यता 50 लाख से भी अधिक लोगों का समूह था। इतनी बड़ी जनसंख्या, जो इस सभ्यता में विकसित 1050 से भी ज्यादा शहरों में बसी थी, के लिए प्रयाप्त मात्रा में अन्न पानी आवास एवं उपयुक्त अभयार्थों का विकास निश्चित रूप से विश्व में प्रथम बार सिंधु घाटी सभ्यता में ही देखने को मिलता है। इस सभ्यता का विकास मानवीय कार्य-शैलता के साथ-साथ अनुकूल जलवायु उपजाऊ मिट्टी घरेलू एवं कृषि कार्य के लिए प्रयाप्त मात्रा में पानी के बिना संभव नहीं था। इतिहासकारों का यह भी मानना है कि जलवायु परिवर्तन एवं नदियों के Hydrological Regime में अनियमित परिवर्तन के कारण ही इस सभ्यता का विनाश हुआ एवं यहाँ के लोग अन्यत्र अनुकूल भौगोलिक परिवेश में प्रवास कर गए।

विस्तार

सिंधु घाटी सभ्यता का विस्तार पश्चिम में बलुचिस्तान से लेकर पूर्व में पश्चिमी, उत्तर प्रदेश तथा उत्तर में उत्तर पूर्वी अफगानिस्तान से लेकर दक्षिण में उत्तरी महाराष्ट्र तक था। प्रारंभ में इस सभ्यता का विस्तार सिंधु नदी घाटी के पश्चिमी छोर तथा बलुचिस्तान के पूर्वी भागों तक ही सीमित था। परन्तु जनसंख्या वृद्धि एवं नए कृषि योग्य भूमि की खोज समुद्रीरास्तों से व्यापार की पश्चिमी क्षेत्रों में प्रतिकूल भौगोलिक (जलवायवीय) परिस्थिति के कारण इस सभ्यता का विस्तार पूर्व एवं दक्षिण में समुद्र तटीय प्रदेशों में हुआ।

भौगोलिक परिस्थिति एवं उसके प्रभाव

किसी भी क्षेत्र विशेष को भौगोलिक परिस्थिति हमेशा एक समान नहीं रहती। भौगोलिक कारक जिनके फलस्वरूप कभी कभी भी मानव सभ्यता का विकास होता है, एक गतिशील तत्व है जो हमेशा बदलते रहे है। सिन्धु घाटी सभ्यता के विकास के कालक्रम में हम देखते हैं कि प्रारंभ में इस सभ्यता का विस्तार सिंधु घाटी क्षेत्र के पश्चिमी जलोढ़ मिट्टी प्रदेश में कृषि प्रधान मानव बस्ती के रूप में हुआ। उस समय इस प्रदेश में प्रयाप्त मात्रा में वर्षा होती थी एवं विभिन्न प्रकार की वनस्पतियाँ पाई जाती थी। यह प्रदेश कृषि के लिए सभी दृष्टिकोण से उपयोगी था।

यहाँ के लागू कृषि के साथ-साथ पशुपालन भी करते थे तथा परिवहन के लिए बैल गाड़ी का उपयोग करते थे। जनसंख्या वृद्धि के साथ अधिक मात्रा में अनाज एवं अन्य सामग्रियों की आवश्यकता हुई। इसी क्रम में इस मानव बस्ती का विस्तार सिंधु घाटी क्षेत्र के मध्य भाग तक हो गया। अनुकूल जलवायु उपजाऊ मिट्टी प्रयाप्त मात्रा में जल की उपलब्धता के कारण कृषि उपज जरूरत से ज्यादा मात्रा में थी। अनाज की अधिकता के कारण इसके संग्रहण एवं जल के क्षेत्रों के क्षेत्रों में निर्यात की आवश्यकता हुई। इसके साथ-साथ अन्य व्यवसायों का भी विकास हुआ। जिसमें व्यापार, कारीगरी, धातुकर्म इत्यादी प्रमुख हैं। व्यावसायिक विशेषज्ञता एवं विशिष्टता के विकास के कारण विभिन्न व्यावसायिक समुदायों में व्यवसाय की शुरुआत हुई। अब कृषक अपना अनाज गैर कृषि क्षेत्रों में संलग्न लोगों को बेचता था। कारीगर अपनी बनाई मूर्तियाँ अन्य क्षेत्रों में बेचता था। इस प्रकार व्यापारी विभिन्न प्रकार की वस्तुओं का संग्रहण कर विभिन्न क्षेत्रों में बेचता था। इस प्रकार के व्यापार के लिए सिंधु घाटी सभ्यता के लोगों ने मुद्रा प्रणाली तथा नापने एवं वजन करने की यूनिट की खोज की। इस तरह छोटे-छोटे सेवा केन्द्रों का विकास हुआ जो की कालांतर में शहर के रूप में परिवर्तित हो गए। सिन्धु घाटी सभ्यता के अवशेषों का अध्ययन करने से यह पता चलाता है कि यहाँ के शहर सुनियोजित तरीके से विकसित किए गए थे। सड़क, जल निकासी, मकान, स्नानघर एवं अन्य जल की अधोसंरचना का विकास जिस तरह से इस सभ्यता के शहरों में देखने को मिलता है, बिना किसी शहरी नियोजन प्राधिकरण के संभव नहीं था। 2600 ई0 पू0 लेकर 1800 ई0 पू0 तक यह सभ्यता अपने सर्वोच्च विकसित स्वरूप में थी। इस अवधि में यहाँ के लोगों ने अन्य नजदीकी सुमेरियन सभ्यता से समुद्र के रास्ते व्यापार भी शुरू किया। अन्य क्षेत्रों में समुद्री रास्ते से व्यापार करने के लिए समुद्र तटीय क्षेत्रों में शहरों का विकास हुआ। ये शहर

शुरूआत में एक व्यापार सामग्री संग्रहण केन्द्र हुआ करते थे। तथा अन्य मुख्य सुविधाओं एवं सेवा के विस्तार के फलस्वरूप ये शहर के रूप में विकसित हुए। इस तरह भौगोलिक परिसर (समुद्र तट एवं सिन्धु नदी के प्रवाह क्षेत्र की आजाऊ मिट्टी) के कारण इस सभ्यता का विस्तार सुदूर दक्षिणी क्षेत्रों में भी हुआ। जलवायुविदों के द्वारा तत्कालीन सिन्धु घाटी क्षेत्र में जलवायु एवं मौसम संबंधी घटनाओं का विस्तृत अध्ययन किया गया। इस अध्ययन में उन्होंने पाया की आज से 5000 वर्ष पहले इस क्षेत्र में मौसम शुष्क होना शुरू हो गया। कालांतर में पानी की कमी हो गई। संभवतः पानी की समस्या के फलस्वरूप शहरों के पास गहन कृषि पद्धति का विकास हुआ। जन-संख्या के अनुसार पर्याप्त मात्रा और सिन्धु की सहायक नदियों की घाटियों में हुआ। पूर्व की ओर के क्षेत्र (आज के सिंधु एवं पंजाब क्षेत्र) में उस समय पर्याप्त मानसुनी वर्षा एवं पदियों के द्वारा जल की उपलब्धता थी जो सिन्धु घाटी सभ्यता के लोगों के लिए एक राहत की बात थी। धीरे-धीरे एवं पंजाब के क्षेत्रों में भी मानसुनी वर्षा कम होती गई और वहाँ के लोग अन्यत्र उपयुक्त क्षेत्र में चले गए। प्रतिकूल जलवायु अर्थातः इस सभ्यता के पतन का कारण बना और इस क्षेत्र के लोग अन्य भौगोलिक क्षेत्र में जा कर बसने के लिए बाध्य हुए।

भौगोलिक कारक-

सिंधु घाटी सभ्यता के विकास एवं पतन के लिए कई भौगोलिक कारक जिम्मेदार थे जिसमें जलवायु, जल विकसित मिट्टी, याताया एवं परिवहन की सुविधा एवं आर्थिक-सामाजिक परिसर प्रमुख थे।

जलवायु - सिंधु घाटी सभ्यता के क्षेत्रों का पुराजलवायविक अध्ययन करने से पता चलता है की प्रारंभ में (7000 ई0पू0) इस क्षेत्र की जलवायु कृषि एवं मानव बस्ती के विकास के लिए आदर्श था। यहाँ पर्याप्त वर्षा एवं सूर्य-प्राप्त होता था जिसके कारण यह क्षेत्र विभिन्न प्रकार के वनस्पतियों एवं जीवों का घर था। कालांतर में परिस्थितिया बदली और धीरे-धीरे यह क्षेत्र भी सुखे के चपेट में आ गया जलवायविक परिस्थितिया पश्चिम से पूर्व के क्षेत्र में ज्यादा अनुकूल थी अतः इस सभ्यता का क्षेत्र विस्तार पूर्व की ओर होता रहा और अंततः प्रतिकूल जलवायु एवं इसमें जमित सुखे ने इस सभ्यता को खत्म कर दिया अतः यह कहा जा सकता है की जलवायविक परिस्थितियों के कारण ही इस सभ्यता का विकास एवं पतन हुआ।

प्रवाह - प्रणाली सिंधु घाटी सभ्यता का नामकरण ही सिंधु नदी के प्रवाह क्षेत्र में होने के कारण इसी नदी के नाम पर हुआ। इस सभ्यता के विकास में सिंधु एवं उसकी सहायक नदियों का महत्वपूर्ण योगदान रहा। किसी भी सभ्यता के विकास के लिए जल की आवश्यकता होती है। सिंधु एवं उसकी सहायक पदियों के द्वारा इस सभ्यता के लोगों को न सिर्फ कृषि, घरेलू एवं अन्य उपयोग के लिए जल प्राप्त हुआ बल्कि इन नदियों के द्वारा लाया गया मलबे बाढ़ के क्षेत्रों में जमा हो कर यहाँ के मिट्टी को निरंतर उपजाऊ बनाती रही। इसी कारण सिंधु घाटी सभ्यता के लोग पर्याप्त मात्रा में अन्न का उत्पादन कर सके।

मिट्टी - टर्सियरी काल में इन्डो-आस्ट्रेलिया प्लेट एवं यूरेशियाई के टकराव के बाद इन दोनों प्लेटों के बीच एक फोरडोप का निर्माण हुआ। इस फोरडोप को कालांतर में नदियों के द्वारा लाए गए मलबे ने भर दिया। सिंधु घाटी सभ्यता का क्षेत्र इसी मलबे से निर्मित जलोढ़ मिट्टी का क्षेत्र है इस क्षेत्र में सिंधु एवं उसकी सहायक नदियों ने क्वार्टररी युग के प्रारंभ से ही जलोढ़ मिट्टी को ला कर जमा किया है। इस क्षेत्र की मिट्टी खास कर नवीनतम जलोढ़ के क्षेत्र अथवा बाढ़ प्रभावित क्षेत्रों की मिट्टी अत्यधिक उपजाऊ रही है। बाद के दिनों में यह क्षेत्र सुखा प्रभावित होने तथा पदियों के Hydriological Regime के परिवर्तन के कारण विश्व के प्रमुख सूखे स्थानों में गिना जाने लगा है। परन्तु यहाँ के उपजाऊ मिट्टी ने ही सिंधु घाटी सभ्यता के विकास की नींव रखी और इसी वजह जनसंख्या के पालन पोषण के लिए अनाज भी उत्पन्न किए।

यातायात एवं परिवहन की सुविधा- सिंधु घाटी सभ्यता के लोगों ने पहिया की खोज कर ली थी या किसी अन्य सभ्यता। इसका ज्ञान प्राप्त कर लिया था। बैल गाड़ी इनके स्थल यातायात का प्रमुख साधन था। इसके माध्यम से इन क्षेत्रों में अनाज, वस्तुओं एवं मानव का परिवहन एक जगह से दूसरे जगह तक संभव था। परिवहन था। परिवहन एवं यातायात की सुविधा के कारण ही यहा के लोग घरेलु एवं विदेशी व्यापार कर रहे थे। परिवहन की अच्छी व्यवस्था एवं सड़कों का विस्तृत जाल एवं समतल मैदान में ही संभव है जो सिंधु घाटी क्षेत्र में सर्वसुलभ था। अतः यहा यातायात एवं परिवहन का पर्याप्त विकास हुआ। इस सभ्यता में कई शहर थे जो अपने पृष्ठ प्रदेश से इस यातायात के व्यवस्था के कारण जुड़े थे और आपस में वस्तु एवं सेवा का आदान प्रदान करते थे। इस सभ्यता के लोगों ने जल यातायात की खोज भी की थी। सिंधु घाटी सभ्यता एवं सुमेरियन सभ्यता में कई दशकों तक व्यापार होता रहा जो मुख्यतः समुद्र के रास्ते अर्थात् अरब सागर से होता था। इस सभ्यता में कई बंदरगाह शहर भी विकसित हुए जो प्रमुख रूप से विदेशी व्यापार के लिए ही बसाए गए थे। जल एवं स्थल यातायात के व्यपक विकास ने इस सभ्यता को आर्थिक रूप से सम्पन्न एवं शहरी सभ्यता बनाया।

आर्थिक एवं सामाजिक परिदृश्य - सिंधु घाटी सभ्यता के लोग शुरूआत में कृषक थे। कृषि पैदावार में बढ़ोतरी एवं जनसंख्या वृद्धि के साथ ही अन्य सुविधाओं की आवश्यकता ने व्यवसायिक विविधीकरण को प्रोत्साहित किया। इस तरह यहा अन्य व्यवसायिक वर्ग जैसे व्यापारी, कारीगर, धातुमर्मिक इत्यादी का उद्भव हुआ। इन व्यवसायों के उद्भव से ही सेवा केन्द्रों का विकास हुआ जो आगे शहरों में परिवर्तित हो गए एवं यह सभ्यता शहरी सभ्यता बनी। इस सभ्यता में व्यापार का महत्व देख कर यह पता चलता है कि व्यापारी यहा के समाज के महत्वपूर्ण लोग होते थे। इस सभ्यता के शहरों की खुदाई से पता चला है की यहा के लोगों को सभी सुविधाएँ समान रूप से मुहैया कराई गई थी परन्तु आर्थिक स्थिति के अनुरूप उनके घर छोटे-बड़े या सुविधा सम्पन्न हुआ करते थे।

निष्कर्ष - सिंधु घाटी सभ्यता विकास भौगोलिक परिस्थितियों के अनुकूल होने के कारण हुआ। कई शतकों तक यह सभ्यता फली-फुली एवं यहा के लोगों का बहुमुखी विकास होता रहा इस क्षेत्र में 5000 वर्ष जलवायु परिवर्तन शुरू हो गया। इसके कारण मानसुनी वर्षा एवं पश्चिम विश्व से प्राप्त वर्षा की मात्रा में कमी आई। इसके साथ-साथ इस क्षेत्र में सुखा का प्रभाव वनस्पतियों एवं जीव जन्तु पर पड़ने लगा। कृषि पैदावार में भी कमी आने लगी। अतः यहा के लोग अधिक वर्षा के क्षेत्र अर्थात् पूर्व की ओर बसने लगे। धीरे-धीरे नए वसे क्षेत्रों में भी सुखा का प्रभाव आ गया। इस तरह इस सभ्यता का पतन हो गया तथा यहा के लोग अन्य क्षेत्रों से जा कर बस गये। इस तरह इस तरह एक महान सभ्यता का अंत हो गया।

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PROBLEMS AND PROSPECT OF BHAGALPUR SILK INDUSTRY

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Abstract: Bhagalpur city is situated in southern Bihar which is part of middle Ganga plain. The city has long history of silk production. Tassar silk made in Bhagalpur is internationally renowned. Weavers in Bhagalpur have been producing Tassar silk since more than 200 years ago. Unfavorable policy of British Government and Political neglect of state and central governments has led to downfall of silk industry in Bhagalpur. This study is aimed to describe history, present condition and future of Bhagalpur silk industry and possibilities for this industry. For this purpose data and information have been collected from different secondary sources and descriptive analysis has been done to find out the results. Descriptive analysis of secondary data and information reveals that Bhagalpur silk industry had a great past when silk produce from Bhagalpur was exported to European and Asian markets. But condition of silk industry in Bhagalpur deteriorated due to unfavorable policy of British government before independence. After independence the industry did not get much support from local and central governments. Further communal riots of 1989 badly affected silk production in Bhagalpur. Since then thousands of weavers lost their looms due to lack of capital, raw material and labor. Once a self dependent weavers were forced to work in giant power looms as labor for minimal payment. Gradually their condition deteriorated and presently production and export of silk from Bhagalpur has reduced significantly. Government measures to rejuvenate silk industry of Bhagalpur are not sufficient and most of these measures have not been implemented properly. The author has suggested creation of large cocoon bank and market linkage to small weavers to uplift the condition of silk industry in Bhagalpur.

METHODOLOGY: This study of silk industry in Bhagalpur is based on secondary data and information which has been collected from different secondary sources. Data and information gathered has been used for descriptive analysis and to find out the result.

RESULT: On the basis of study of condition of silk industry in Bhagalpur the author has found that the industry is in critical condition which was once lifeline of the silk city. Reason behind its deterioration is mainly political neglect of local silk industry and social tension in the study area. The condition of this industry can be uplifted with proper implementation of government measures.

CONCLUSION: Since ancient times Bhagalpuri silk has been famous for its softness and comfort. The silk industry in the study area has witnessed rise before independence and fall after 1990s. the deteriorating silk industry in the silk city has put local weavers in measurable condition. Now most of them live below poverty line. The condition of silk industry of Bhagalpur can be uplifted with some strict measures and its proper implementation.

INTRODUCTION:

Silk is one of the most important fabrics for textile production in the world. Silk is used for production of blanket, chadar, dupattah, scarves, stoles, sari and other dress materials. India is second largest producer of silk in the world after China. India produces 30000 tonnes of raw silk every year which is 18% of total production of raw silk in the world. India produces five types of

raw silk i.e. Mulberry silk, Vanya silk, Tassar silk, Eri silk and Muga silk. Silk industry in India employs 82.5 lakh populations. In year 2017-18 India exported silk worth of 2800 crores. Important silk producing states in India are Karnataka, Andhra Pradesh, Assam, West Bengal, Jharkhand, Tamilnadu, Meghalaya, Nagaland, Manipur and Maharashtra. Bihar is 23rd largest silk producing state in India which accounts for 9 metric tonnes of raw silk (2017-18) production. Bhagalpur in Bihar is only significant producer of silk in the state. The city is producing silk since 200 years ago. Once, bank of river Ganga from Bhagalpur to Munger was flooded with weavers who used to produce silk thread and silk textile for local and international market. Tassar silk produced in this belt has been internationally renowned for its softness and comfort. The city has been named as Silk City due to its ancient tradition of silk manufacturing. There are four clusters of silk production in Bhagalpur i.e. Hussainabad, Nathnagar, Champanagar and Kharik Bazar. There are more than 25000 handlooms and 100 units of power loom in the city. Two million meters of silk is produced in the city per year. Total trade of silk from Bhagalpur is about 100 crores per year out of which fifty percent is exported to international market. About one lakh population in Bhagalpur city is engaged in silk production. Silk textile from Bhagalpur is famous in local as well as Arabian, European and American markets.

OBJECTIVE AND METHODOLOGY:

This study is aimed to describe the temporal changes in silk industry of Bhagalpur. This research also briefly describes the hurdles in development of silk industry in Bhagalpur. The study also incorporates possible measures to uplift the deteriorating silk industries in the study area. For descriptive study of silk industry in the study area secondary data and information has been collected from different secondary sources. Data and information gathered has been used for descriptive analysis and to find out the result.

PROBLEMS OF SILK INDUSTRY IN BHAGALPUR:

Once a flourishing silk industry of Bhagalpur deteriorated gradually due to several factors such as increasing cost of raw materials, competition from cheap silk of other states and imported cheap silk or mixed silk textile, lack of working capital, lack of marketing support, shortage of yarn, migration of weavers and labourer, erratic power supply, competition from highly productive power looms. Bhagalpur silk industry had witnessed its zenith before independence of India. Due to faulty policies in colonial regime and political negligence of contemporary governments the industry is gradually proceeding towards the nadir. In 1992 about thirty lakh population in Bhagalpur were dependent on silk industry. There were two lakhs of weavers engaged in production of silk in Bhagalpur. Total annual turnover from silk manufacturing and trade was about 500 crores in 1992 (Asian Age, 9th June 2017). The number of weavers decreased to 35000 in year 2000 and 17000 in 2007. In year 2000 total turnover of silk industry in Bhagalpur reduced to 100 crores which further decreased to 60 crores in 2008 (Hindustan Times, 1st September 2009). In consequence to critical condition of silk industry in the study area many handloom owners turned to labourer, now working for other giant power looms or work for traders and middleman. Problems of silk industry of Bhagalpur have been discussed in brief in following paragraphs.

Increasing cost of raw material –

Weavers of Bhagalpur are facing problem of shortage of raw material for silk production. Due to shortage of raw material its price is increasing day by day. Increasing price of raw material has led to closure of many small handloom mills in the study area. Further, small weavers who cannot

not afford to buy costly raw material buy mixed silk yarn or smuggled silk yarn from China and South Korea. So quality of silk textile from their mill is low and these weavers get lower price for their product.

Competition from other states –

Though Bhagalpur silk industry is crisis phase, other silk producing centers like Bangalore, Ahmadabad, Mumbai etc. are flourishing due to high profit from export and sell in domestic market. These centers are tough competitor for small weavers of Bhagalpur. Further huge centers of silk production get skilled labourer from Bhagalpur, who were once handloom owners in the study area and migrated to these centers due to closure of their enterprise.

International competition –

Silk industry of Bhagalpur is facing tough competition from cheap silk yarn and silk textile. Countries like China and South Korea are major silk producing centers. China is the largest producer and exporter of silk in the world. India also imports silk from China and South Korea. Imported silk are cheaper than silk produced in Bhagalpur so weavers of Bhagalpur are not able to replace imported silk from these Asian giants. Further weavers of the study area are forced to buy imported yarn or smuggled yarn from China and South Korea as these are cheaper than locally produced silk yarn.

Lack of working capital –

Silk industry of Bhagalpur comes under cottage industry as most of the manufacturing units are small handloom units with less than 20 looms and low investment. Weavers are average people. Most of them are below poverty line and do not have much capital to invest. They do not get financial support from Banks to increase their working capital for more production. Banks in spite of Government order regarding loan sanction to weavers, do not provide loan to small weavers. Most of the loans are sanctioned to large mills which already have enough working capital for their growth. In these conditions small weavers get loan from local market at very high interest rate of more than 5% per month. So, production cost of silk for small weavers is quite high and thus profit is low for small weavers.

Shortage of yarn –

Silk industry in Bhagalpur is facing problem of shortage of yarn. Due to shortage of yarn its cost is increasing and it has become difficult for small weavers to buy good quality silk yarn. So, small weavers depend upon imported or smuggled silk yarn from South Korea and China or mixed low quality yarn.

Lack of marketing support –

Small silk weavers of Bhagalpur are not able to sell their products due to lack of market connection and supports. Most of the small weavers are dependent on middlemen and traders for sell of their manufactured textile. Weavers get very low price for their product from middlemen and traders. Same product is sold by traders and middlemen at high cost and their profit margin is quite higher than that of weavers. So, silk production is not profitable business for these small weavers.

Social problem (communal riot) –

Most of the silk weavers in Bhagalpur belong to particular community (Muslim). In year 1989 many small handloom mills were burnt during communal riot in Bhagalpur. This incident badly affected production of silk in the silk city. Most of the weavers never regained their profitable business and turned as labourer who get only 50 rupees for one meter of silk cloth production. Few of them turned to vegetable seller and few of them migrated to other state to work as labourer in mills.

Migration of weavers and labourer –

Silk industry of Bhagalpur deteriorated due to political negligence of governments. Communal riot of 1989 further enhance the problems of this industry. Silk production has not remained profitable for weavers and youth labourers. Most of them migrated to other textile centers such as Surat, Ahmedabad, Bangalore and Mumbai. Critical condition of silk industry in Bhagalpur has become more pronounced due to migration of skilled labourer and weavers from the silk city.

Erratic power supply –

Bhagalpur gets power supply of less than ten hours a day. Power fluctuation and low voltage are other associated problems of power supply in Bhagalpur city. Due to low power supply production of silk is affected badly. Most of the power looms run on generator so cost of production increases for them. Further subsidy from state government to weavers for power supply is not distributed properly. Most of the small weavers do not get these subsidies. Government assurance of remittance of power bill for small weavers is still on paper.

High input cost –

Input cost for silk industry is much higher in Bhagalpur due to some local circumstances. Cost of raw material for silk production is quite high in Bhagalpur so weavers either buy cheap imported or smuggled raw material. There is less than ten hour of power supply in the study area. Voltage fluctuation and low voltage are other problems associated with power supply in the study area. Due to problem associated with power supply looms use generator for continuous power supply. Most of the skilled labourer migrated to other silk centers of India so labour cost has also increased in the study area. In these circumstances input cost of silk industry in Bhagalpur is quite higher in comparison to other silk centers of the country.

Low productivity –

Most of the silk produce in Bhagalpur comes from small handlooms where tradition machines and methods of production are still used. Productivity of these looms is very low in comparison to power looms and rejuvenated handloom centers. Due to low productivity of handlooms in Bhagalpur weavers get less profit and low demand from market.

Competition from cheap mixed silk fabric –

Cost of local made silk yarn in the city is very high. Recently mixed silk fabric has flooded the market due to its low cost and affordability for middle and lower class. Mixed silk fabric looks alike to tassar silk of Bhagalpur but its quality is lower than that of original Bhagalpur silk. Due to low cost of textile made from mixed silk fabric its demand is high in market and so weavers of original Bhagalpuri silk are forced to either sell their product at low cost or used mixed silk fabric for textile production.

Covid 19 Blast-

Present corona outbreak has led to return of migrants from different states to their home in Bhagalpur. So burden on low income weavers family has increased. Now most of their saving is utilized in rearing of their wards and they have very little to invest in their business.

GOVERNMENT MEASURES FOR DEVELOPMENT:

Government of India together with the state government has initiated several programmes for development of silk industry in Bhagalpur. Measures taken by the governments for its development are; provision of supporting infrastructure, silk worm rearing appliances, host plantation, financial support through banks and subsidized power supply. Further Government of India announced support for silk industry in Bhagalpur through setting up one big cluster with capacity of 5000 looms which will be composed of five small clusters and one mega handloom cluster. Government of India also announced establishment of Basic Seed Multiplication and

Training Center (BSMTC) for production and supply of good quality Tassar seeds. Demonstration cum Technical Center (DTC) and Tassar Seed Bank (TSB) are also to be established by the Central Government. These measures of development of silk industry in Bhagalpur are not sufficient and these are unable to uplift the critical condition of silk industry in the study area. The main reason behind unsuccessfulness of these measures is improper implementation of these programmes by middlemen.

SUGGESTIONS:

The deteriorating condition of silk industry in Bhagalpur is critical for weavers in the silk city. Weavers in the study area are totally dependent on silk industry for their livelihood. The critical condition of silk industry in Bhagalpur has put weaver's life on risk and most of them now live below poverty line. So, there is an urgent need to uplift the condition of silk industry in the study area. Viewing the condition of silk industry in the study area author suggests setting up of Co-operative Tassar Seed Bank (CTSB) and financial support to small weavers for upliftment of silk industry and condition of small weavers in the study area.

CONCLUSION:

Silk industry of Bhagalpur is lifeline of weavers in the study area. Silk production in the study area has been main occupation of local urbanites since more than two hundred years. Silk produced in the study area is of superior quality. Bhagalpuri silk is famous in domestic and international market. It has been exported to European and American market since colonial period. Today condition of silk industry in the study area is deteriorating and its condition has become critical. The main reason behind downfall of silk industry in the study area is political neglect of the silk industry of Bhagalpur. The condition of weavers in the study area and silk industry of Bhagalpur can be uplifted by some measures like development of seed bank by local entrepreneur and financial support to weavers. Rejuvenation of silk industry in the study area will not only uplift the condition of weavers but it will also uplift the local economy.

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