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MESSAGE FROM EDITORS' DESK

It gives us an immense pleasure in bringing out the sixth volume of International Journal of Science and Humanities with your incessant support. International Journal of Science and Humanities being published by Islamiah College has been successfully marching towards its sixth year by providing a platform for authors in exhibiting their talents in the form of their research articles on various disciplines such as English, Chemistry, Bio-Chemistry, Commerce, Management, History, Sociology, Public Administration, Political Science, Physics, Economics and Mathematics.

Since it is the International Journal, we are invariably committed to do our best by ensuring that the articles published by the authors of various disciplines are free from error, plagiarism and biased. However, we will never compromise on the quality of journal as our journal is subjected to peer review. All the papers of different disciplines are thoroughly scrutinised by our peer review members who are employed in various reputed institutions all over the world.

Therefore, we humbly request you to provide your valuable suggestions in further strengthening this Journal and always extend your support by publishing your quality articles in our reputed International Journal of Science and Humanities.

Disclaimer

APPEAL

I am delighted to introduce this issue of International Journal of Science and Humanities (IJSH) to the students and research community on behalf of Islamiah College (Autonomous), Vaniyambadi, a century old institution serving for the cause of education to socially, economically and educationally weaker sections of the society. The IJSH, is a peer reviewed research journal of interdisciplinary nature that cater the needs of the teaching and research society. The aim of the journal is not only to provide a space for leading research work but also provide a platform for the budding researchers to publish their maiden attempt in the field of science and humanities. The objective of IJSH is to publish up-to-date, high-quality and original research papers alongside relevant and insightful reviews.

The initiative to start this journal was taken by Janab L.M Muneer Ahmed, the Secretary & Correspondent of this College with an aspiration to keep the research vibrant in this campus. Now, the torch is handed over to me from June 2016 onwards to run this journal on non-profitable basis without compromising its aims and objectives. At this juncture, I appeal to all teaching and research communities to concentrate on both teaching and research relevant to society, which are symbolically related as the two faces of the same coin. I also appeal to all reviewers and editors not to compromise with the quality of the input and promote this journal to the next level with excellent output. Finally, I pray Almighty to provide guidance for development and success of this journal. Best wishes and thanks for your contribution to the IJSH.

Mr. L.M. MUNEER AHMED
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TESTING BNBRU AGEING CLASS OF LIFE-TIME DISTRIBUTION BASED ON MOMENT INEQUALITY

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Abstract

In this paper, a new moment inequality is derived for Bivariate New Better than Renewal Used (BNBRU) ageing class of life-time distribution. This inequality demonstrates that if the mean life is finite, then all higher order moments exist. Based on the Moment inequality, new testing procedures for testing bivariate exponentiality against BNBRU ageing class of life-time distribution is introduced. The asymptotic normality of the test statistic and its consistency are studied. Using Monte Carlo Method, critical values of the proposed test are calculated for $n = 5(5)100$ and tabulated. Finally, the theoretical results are applied to analyze real-life data sets.

Keywords: Classes of Life-Time Distribution, BNBRU, Moment Inequality, U-Statistic and Life Testing.

1. Introduction

Certain classes of life-time distributions and their variations have been introduced in reliability theory, the applications of these classes of life-time distributions can be seen in engineering, biological science, maintenance and biometrics. The main aim of constructing new tests is to gain higher efficiencies.

Testing bivariate exponentiality against some bivariate ageing classes of life-time distributions has seen a good deal of attention. The moment inequality for the Bivariate New Better than Renewal Used (BNBRU) ageing class of life-time distribution can be found in the work of Sathiyaraj and Rizwan (2019). Now we propose a test statistic for testing Bivariate Exponentiality Against Bivariate New Better than Renewal Used (BNBRU) ageing class of life-time distribution, based on the moment inequality.

The rest of the paper is arranged as follows; In section 2, the preliminaries required for the further discussion are given. In section 3, moment inequality for the Bivariate New Better than Renewal Used (BNBRU) ageing class of life-time distribution is derived. A new test statistic for testing Bivariate New Better than Renewal Used (BNBRU) ageing class of life-time distribution based on moment inequality is proposed in section 4. Using Monte Carlo Method, critical values of the proposed test statistic are calculated for $n = 5(5)100$ and tabulated in section 5. The application of the proposed test to real data sets is discussed in section 6. Finally, conclusion is given in section 7.

2. Preliminaries

Let (X, Y) denote the survival time of a device having a joint distribution function $F(x, y)$. The bivariate joint survival function is given by

$$\overline{F}(x, y) \quad = \quad P(X > x, Y > y), \qquad x, y \geq 0$$

where it is assumed that $\overline{F}(0, 0) = 1$.
The following definition of Bivariate ageing classes of life-time distributions appeared in Sathiyaraj and Rizwan (2019).

Definition 2.1. *A bivariate random variable* (X, Y) *or its distribution* $\overline{F}(x, y)$ *is said to have Bivariate New Better than Renewal Used (BNBRU) ageing class, if*

$$\overline{W}(x + t, y + s) \leq \overline{F}(x, y)\overline{W}(t, s),$$

for all $x, y, t, s \geq 0$, *where*

$$\overline{W}(x, y) = \frac{1}{\mu} \int_x^\infty \int_y^\infty \overline{F}(u, v) dv du,$$

$\mu = \int_0^\infty \int_0^\infty \overline{F}(x, y) dy dx$ *denotes the mean of* F *and is assumed to be finite.*

Definition 2.2. *The r-th Moment of a bivariate random variable* (X, Y) *is*

$$\mu_r = E(X^r Y^r) = r^2 \int_0^\infty \int_0^\infty (xy)^{r-1} \overline{F}(x, y) dy dx.$$

3. Moment Inequality

A moment inequality is derived for the system whose life-time distribution is a Bivariate New Better than Renewal Used ageing class of life-time distribution.

Theorem 3.1. *If F is a Bivariate New Better than Renewal Used ageing class of life-time distribution, and its $(r+3)$-rd moments is finite, for some integer $r \geq 0$, then*

$$\frac{\mu_{r+3}}{(r+2)(r+3)} \leq \sum_{i=0}^{r} \binom{r}{i} \frac{\mu_{i+1}\mu_{r-i+2}}{(i+1)(r-i+1)(r-i+2)}.$$

Proof. Since F is a Bivariate New Better than Renewal Used ageing class of life-time distribution, we have

$$\overline{W}(x+t, y+s) \leq \overline{F}(x,y)\overline{W}(t,s),$$

for all $x, y, t, s \geq 0$, where

$$\overline{W}(x,y) = \frac{1}{\mu}\int_x^\infty \int_y^\infty \overline{F}(u,v)dvdu,$$

Multiplying both side by $(x+t)^r(y+s)^r$ and integrating, we get

$$\begin{aligned}\int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty (x+t)^r(y+s)^r \overline{W}(x+t,y+s)dydxdsdt \\ \leq \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty (x+t)^r(y+s)^r \overline{F}(x,y)\overline{W}(t,s)dydxdsdt \quad (3.1)\end{aligned}$$

On Substituting $x+t = z_1$ and $y+s = z_2$, the left side of the inequality becomes

$$\begin{aligned}&\int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty (x+t)^r(y+s)^r \overline{W}(x+t,y+s)dydxdsdt \\ &= \int_0^\infty \int_0^\infty \int_s^\infty \int_t^\infty (z_1z_2)^r \overline{W}(z_1,z_2)dz_1dz_2dtds \\ &= \int_0^\infty \int_0^\infty (\alpha\beta)^r \overline{W}(\alpha,\beta) \int_0^\alpha \int_0^\beta dz_1dz_2d\alpha d\beta \\ &= \int_0^\infty \int_0^\infty (\alpha\beta)^{r+1} \overline{W}(\alpha,\beta)d\alpha d\beta \\ &= \frac{1}{\mu}\int_0^\infty \int_0^\infty (\alpha\beta)^{r+1} \int_\beta^\infty \int_\alpha^\infty \overline{F}(u,v)dvdud\alpha d\beta \\ &= \frac{1}{\mu}\int_0^\infty \int_0^\infty \overline{F}(u,v) \int_0^u \int_0^v (\alpha\beta)^{r+1} dvdud\alpha d\beta \\ &= \frac{1}{\mu}\int_0^\infty \int_0^\infty \frac{(uv)^{r+2}}{r+2}\overline{F}(u,v)dvdu \\ &= \frac{\mu_{r+2}}{\mu(r+2)(r+3)} \quad (3.2)\end{aligned}$$

and

$$\begin{aligned}
&\int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty (x+t)^r (y+s)^r \overline{F}(x,y)\overline{W}(t,s)dydxdsdt \\
&= \sum_{i=0}^{r} \binom{r}{i} \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty x^i\, t^{r-i}\, y^i\, s^{r-i}\, \overline{F}(x,y)\overline{W}(t,s)dydxdsdt \\
&= \sum_{i=0}^{r} \binom{r}{i} \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty x^i\, t^{r-i}\, y^i\, s^{r-i}\, \overline{F}(x,y)\overline{W}(t,s)dydxdsdt \\
&= \sum_{i=0}^{r} \binom{r}{i} \left[\left(\int_0^\infty \int_0^\infty (xy)^i \overline{F}(x,y)dydx\right)\left(\int_0^\infty \int_0^\infty (ts)^{r-i}\overline{W}(t,s)dsdt\right)\right] \\
&= \sum_{i=0}^{r} \binom{r}{i} \frac{\mu_{i+1}}{(i+1)} \left[\frac{1}{\mu}\int_0^\infty \int_0^\infty (ts)^{r-i} \int_s^\infty \int_t^\infty \overline{F}(u,v)dvdudsdt\right] \\
&= \sum_{i=0}^{r} \binom{r}{i} \frac{\mu_{i+1}}{(i+1)} \frac{1}{\mu}\int_0^\infty \int_0^\infty \overline{F}(u,v) \int_0^s \int_0^t (uv)^{r-i} dvdudsdt \\
&= \sum_{i=0}^{r} \binom{r}{i} \frac{\mu_{i+1}}{(i+1)} \frac{1}{\mu}\int_0^\infty \int_0^\infty \frac{(ts)^{r-i+1}}{(r-i+1)} \overline{F}(t,s)dsdt \\
&= \frac{1}{\mu}\sum_{i=0}^{r} \binom{r}{i} \frac{\mu_{i+1}}{(i+1)} \frac{1}{\mu} \frac{\mu_{r-i+2}}{(r-i+1)(r-i+2)} \qquad (3.3)
\end{aligned}$$

Using the equations (3.2) and (3.3), the inequality (3.1) becomes

$$\frac{\mu_{r+2}}{(r+2)(r+3)} \leq \sum_{i=0}^{r} \binom{r}{i} \frac{\mu_{i+1}}{(i+1)} \frac{\mu_{r-i+2}}{(r-i+1)(r-i+2)}. \qquad (3.4)$$

This completes the proof of theorem. □

4. Testing Bivariate Exponentiality against Bivariate New Better than Renewal Used Ageing Class

Using inequality (3.4), we test the null hypothesis

$H_0 : F$ is Bivariate exponential

against the alternative hypothesis

$H_1 : F$ is BNBRU and not bivariate exponential.

Consider the bivariate exponential distribution introduced by Marshall and Olkin (1967), given by

$$\overline{F}(x, y) = \exp(-\lambda_1 x - \lambda_2 y - \lambda_{12} \max(x, y)),$$

for all $x, y, \lambda_1, \lambda_2 > 0$ *and* $\lambda_{12} \geq 0$, where

$$\begin{aligned}
\lambda_1 &= \frac{\mu_1 + \mu_2}{\mu_{12}} - \frac{1}{\mu_2} \\
\lambda_2 &= \frac{\mu_1 + \mu_2}{\mu_{12}} - \frac{1}{\mu_1} \\
\lambda_{12} &= \left(\frac{1}{\mu_1} + \frac{1}{\mu_2}\right) \frac{\mu_{12} - \mu_1 \mu_2}{\mu_{12}} \\
\mu_1 &= \int_0^\infty \overline{F}(x, 0) dx \\
\mu_2 &= \int_0^\infty \overline{F}(0, y) dy
\end{aligned}$$

and

$$\mu_{12} = \int_0^\infty \int_0^\infty \overline{F}(x, y) dx dy.$$

Define

$$\delta_E = \sum_{i=0}^{r} \binom{r}{i} \frac{\mu_{i+1} \mu_(r - i + 2)}{(i + 1)(r - i + 1)(r - i + 2)} - \frac{\mu_{r+3}}{(r + 2)(r + 3)} \tag{4.1}$$

Note that under H_0, $\delta_E = 0$, while under H_1, $\delta_E > 0$. Let $(X_1, X_2), (X_3, X_4), \ldots, (X_{i-1}, X_i)$, $\ldots (X_{n-1}, X_n)$ be a bivariate random sample from a distribution F.

Taking $r = 1$ in equation (4.1), we get

$$\delta_E = \frac{1}{6} \mu \, \mu_3 + \frac{1}{4} \mu_2^2 - \frac{1}{12} \mu_4$$

The estimate $\widehat{\delta_E}$ of δ_E can be obtained as

$$\widehat{\delta_E} = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \phi(X_i, X_j),$$

where

$$\phi(X_i, X_j) = \frac{1}{6} X_i \, X_j^3 + \frac{1}{4} X_i^2 \, X_j^2 - \frac{1}{12} X_j^4.$$

To make the test statistic scale invariant, let

$$\begin{aligned}\widehat{\Delta}_E &= \frac{\widehat{\delta}_E}{\mu^4} \\ &= \frac{1}{\mu^4}\left[\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\frac{1}{6}X_i\,X_j^3+\frac{1}{4}X_i^2\,X_j^2-\frac{1}{12}X_j^4\right)\right]\end{aligned}$$

Then $\widehat{\Delta}_E$ is equivalent to the classical U-statistic, [Lee(1989)] and is given by

$$U_n = \frac{1}{\binom{n}{2}}\sum_{i<j\,\leq n}\phi(X_i,X_j).$$

The asymptotic normality of $\widehat{\Delta}_E$ is summarized in the following theorem.

Theorem 4.1. *As* $n\to\infty$, $\sqrt{n}\,(\widehat{\Delta}_E-\delta_E)$ *is asymptotically normal with mean zero and variance* σ^2, *where*

$$\sigma^2 = Var\left\{\frac{1}{6}X_i^2\,\mu_3+\frac{1}{4}X_i^2\,\mu_2-\frac{1}{12}\mu_4\;+\frac{1}{6}\,\mu\,X_j^3+\frac{1}{4}\mu_2X_j^2-\frac{1}{12}X_j^4\right\}.$$

Under H_0, *the variance reduces to* $\sigma^2 = 102$.

Proof. From the standard theory of U-statistic, Lee(1989), we have

$$\sigma^2 = Var\{\varsigma(X_i,X_j)\},$$

where

$$\begin{aligned}\varsigma(X_i,X_j) &= E[\phi(X_i,X_j)\mid X_i]+E[\phi(X_i,X_j)\mid X_j] \\ E[\phi(X_i,X_j)\mid X_i] &= \frac{1}{6}X_i^2\,\mu_3+\frac{1}{4}X_i^2\,\mu_2-\frac{1}{12}\mu_4 \\ E[\phi(X_i,X_j)\mid X_j] &= \frac{1}{6}\,\mu\,X_j^3+\frac{1}{4}\mu_2X_j^2-\frac{1}{12}X_j^4\end{aligned}$$

and

$$\varsigma(X_i,X_j) = \frac{1}{6}X_i^2\,\mu_3+\frac{1}{4}X_i^2\,\mu_2-\frac{1}{12}\mu_4\;+\frac{1}{6}\,\mu\,X_j^3+\frac{1}{4}\mu_2X_j^2-\frac{1}{12}X_j^4.$$

Thus

$$\sigma^2 = Var\left\{\frac{1}{6}X_i^2\,\mu_3+\frac{1}{4}X_i^2\,\mu_2-\frac{1}{12}\mu_4\;+\frac{1}{6}\,\mu\,X_j^3+\frac{1}{4}\mu_2X_j^2-\frac{1}{12}X_j^4\right\}.$$

Under H_0,

$$\varsigma_0(X_i, X_j) \;=\; X_i + \frac{1}{2}(X_i^2 + X_j^2) + \frac{1}{6}X_j^3 \; - \frac{1}{12}\; X_j^4 - 2. \tag{4.2}$$

From the equation (4.2), it is clear that $E[\varsigma_0(X_i, X_j)] = 0$ and

$$\sigma^2 = E[(\varsigma_0(X_i, X_j))^2] = 102.$$

This completes the proof of the theorem. □

Corollary 4.1. *Under H_0, the limiting distribution of U_n is normal with mean $\widehat{\Delta}_E$. The variance of $\sqrt{n}(U_n)$ is a function of λ_1, λ_2 and λ_{12}.*

Proof. Since the variance of $\sqrt{n}(U_n)$ is very complicated under H_0 and since U_n is a function of U -statistic, jackknifing would not only reduce the bias, but also enable us to estimate the variance of $V(\sqrt{n}U_n)$.

The estimate of $V(\sqrt{n}U_n)$ is

$$\widehat{V}(\sqrt{n}U_n) \;=\; \frac{n}{n-1}\sum_{i=1}^{n}[U_{n,i} - U_n^*]^2$$

where

$$U_{n,i} = U_{n-1}(X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_n)$$

and

$$U_n^* = \frac{1}{n}\sum_{i=1}^{n} U_{n,i}.$$

Using the results from Sen (1977), $\dfrac{\sqrt{n}(U_n)}{[\widehat{V}(\sqrt{n}U_n)]^{\frac{1}{2}}}$ is asymptotically standard normal.

Thus $\dfrac{\sqrt{n}(U_n)}{[\widehat{V}(\sqrt{n}U_n)]^{\frac{1}{2}}} \;\sim\; N(0,1)$.

This completes the proof of the corollary. □

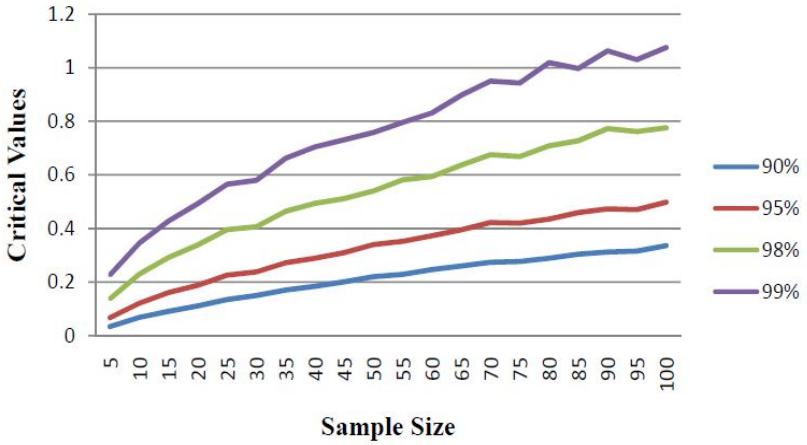
5. Monte Carlo Simulations

In this section, the Monte Carlo null distribution critical points of $\widehat{\Delta}_E$ are simulated based on 25000 generated samples of size $n = 5(5)100$. Table 1 gives the upper percentile points of statistic $\widehat{\Delta}_E$ for different confidence levels 90%, 95%, 98% and 99%.

Table 1. Critical Values of the statistic $\widehat{\Delta}_E$

n	90%	95%	98%	99%
5	0.034	0.067	0.138	0.227
10	0.068	0.121	0.230	0.346
15	0.091	0.161	0.292	0.428
20	0.111	0.188	0.339	0.493
25	0.135	0.226	0.396	0.565
30	0.150	0.238	0.407	0.580
35	0.170	0.272	0.464	0.662
40	0.184	0.289	0.494	0.704
45	0.201	0.310	0.512	0.731
50	0.220	0.340	0.540	0.758
55	0.229	0.352	0.582	0.796
60	0.247	0.373	0.594	0.831
65	0.260	0.395	0.637	0.897
70	0.274	0.422	0.676	0.950
75	0.277	0.420	0.669	0.943
80	0.289	0.435	0.709	1.019
85	0.304	0.459	0.728	0.997
90	0.312	0.473	0.773	1.063
95	0.316	0.470	0.762	1.030
100	0.336	0.498	0.776	1.075

Figure 1: Relation between critical values and sample size for different confidence levels



It is clear from Table 1 and Figure 1, that the critical values increase as the confidence level increases and almost increases as the sample size increase.

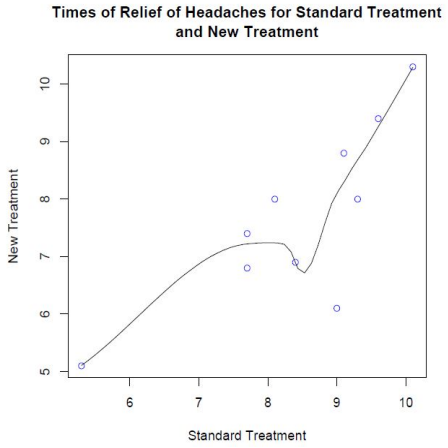
6. Application to Real Life Data

In this section, we consider an example given by Gross and Clark(1975). The data are given in Table 2 which denotes the length of time required for patients with headaches to achieve relief; each patient receives a standard treatment and a new treatment on separate occasions. The times are recorded to the nearest tenth of a minute. This table appeared in Gross and Clark (1975, p. 232). We use our test to detect whether these times of relief of headaches for standard and new treatment (Minutes) follow a bivariate exponential distribution with exponential minimum.

Table 2. Times of Relief of Headaches for Standard Treatment and New Treatment (Minutes)

Patient	Standard Treatment	New Treatment
1	8.4	6.9
2	7.7	6.8
3	10.1	10.3
4	9.6	9.4
5	9.3	8.0
6	9.1	8.8
7	9.0	6.1
8	7.7	7.4
9	8.1	8.0
10	5.3	5.1

Figure 2: Graph of Relief of Headache for Standard Treatment and New Treatment



Using the data in Table 2, we obtain, the value of the test statistic $\widehat{\Delta}_E = 0.002518519$. Thus $\dfrac{\sqrt{n}(U_n)}{[\widehat{V}(\sqrt{n}U_n)]^{\frac{1}{2}}} = 15.6562059454$.

Hence, we reject H_0 and conclude in favour of BNBRU. Then we accept H_1 which shows that the data set has Bivariate New Better than Renewal Used property, but not Bivariate exponential.

7. Conclusion

The Bivariate New Better than Renewal Used Ageing Class of life-time distribution is considered. The moment inequality is derived. A new test statistic for testing Bivariate Exponentiality against Bivariate New Better than Renewal Used ageing class of life-time distributions based on the moment inequality is proposed. Using Monte Carlo Method, critical values of the proposed test are calculated for $n = 5\ (5)\ 100$ and tabulated. Finally, application to real-life data is given.

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A STUDY ON ANTI-FUZZY NORMAL SUBNEARRINGS

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Abstract

In this paper, we made an attempt to study the algebraic nature of fuzzy normal subnearring and its properties.

Keywords: Fuzzy Set, Fuzzy Subnearring and Anti-Fuzzy Normal Subnearring.

1. Introduction

There are many concepts of universal algebras generalizing an associative ring $(R; +, .)$. Some of them in particular, near rings and several kinds of semi rings have been proven very useful. An algebra $(R; +, .)$ is said to be a near ring if $(R, +)$ is a group and $(R, .)$ are semi group satisfying $a.(b + c) = a.b + a.c$, for all a, b and c in R. After the introduction of fuzzy sets by L.A.Zadeh, several researchers explored on the generalization of the concept of fuzzy sets. The notion of Fuzzy subnear rings and ideals was introduced by S.Abou Zaid. In this paper, we introduce anti-fuzzy normal subnearring of a near ring and prove some properties.

2. Properties of Anti-Fuzzy Normal Subnearrings

Definition 2.1. *Let R be a nearring. A fuzzy subset A of R is said to be an anti-fuzzy subnearring (AFSNR) of R if it satisfies the following conditions:*

(i) $\mu_A(x - y) \leq \max\{\mu_A(x), \mu_A(y)\}$,

(ii) $\mu_A(xy) \leq \max\{\mu_A(x), \mu(y)\}$, *for all x and y in R.*

Definition 2.2. *Let R be a nearring. An anti-fuzzy subnearring A of R is said to be a anti-fuzzy normal subnearring (AFNSNR) of R if it satisfies the following conditions:*

(i) $\mu_A(x+y) = \mu_A(y+x)$,

(ii) $\mu_A(xy) = \mu_A(yx)$, *for all x and y in R.*

Theorem 2.1. *Let* $(R, +, \cdot)$ *be a near ring. If A and B are two anti-fuzzy normal subnearrings of R, then their union* $A \cup B$ *is an anti-fuzzy normal subnearring of R.*

Proof. Let x and y in R. Let $A = \{\langle x, \mu_A(x)\rangle / x \in R\}$ and $B = \{\langle x, \mu_B(x)\rangle / x \in R\}$ be anti-fuzzy normal subnearrings of a nearring R.
Let $C = A \cup B$ and $C = \{\langle x, \mu_C(x)\rangle / x \in R\}$.
Clearly C is an anti-fuzzy subnearring of a nearring R,
Since A and B are two anti-fuzzy subnearrings of a nearring R. And,

$$\begin{aligned}\mu_C(x+y) &= \max\{\mu_A(x+y), \mu_B(x+y)\},\\ &= \max\{\mu_A(y+x), \mu_B(y+x)\},\\ &= \mu_C(y+x)\end{aligned}$$

Therefore, $\mu_C(x+y) = \mu_C(y+x)$, for all x and y in R. Also

$$\begin{aligned}\mu_C(xy) &= \max\{\mu_A(xy), \mu_B(xy)\},\\ &= \max\{\mu_A(yx), \mu_B(yx)\},\\ &= \mu_C(yx)\end{aligned}$$

Therefore, $\mu_C(xy) = \mu_C(yx)$, for all x and y in R.
Hence $A \cup B$ is an anti-fuzzy normal subnearring of a nearring R. □

Theorem 2.2. *Let R be a nearring. The union of a family of anti-fuzzy normal subnearrings of R is an anti-fuzzy normal subnearring of R.*

Proof. Let $\{A_i\}_{i\in I}$ be a family of anti-fuzzy normal subnearrings of a nearring R and let $A = \bigcup_{i\in I} A_i$.
Then for x and y in R.
Clearly the union of a family of anti-fuzzy subnearrings of a nearring R is an anti-fuzzy subnearring of a nearring R.
(i)

$$\begin{aligned}\mu_A(x+y) &= \sup_{i\in I}\mu_{A_i}(x+y)\\ &= \sup_{i\in I}\mu_{A_i}(y+x)\\ &= \mu_A(y+x)\end{aligned}$$

Therefore, $\mu_A(x+y) = \mu_A(y+x)$ for all x and y in R.

(ii)
$$\begin{aligned}\mu_A(xy) &= \sup_{i\in I}\mu_{A_i}(xy)\\ &= \sup_{i\in I}\mu_{A_i}(yx)\\ &= \mu_A(yx)\end{aligned}$$

Therefore, $\mu_A(xy) = \mu_A(yx)$ for all x and y in R.

Hence the union of a family of anti-fuzzy normal subnearrings of a nearring R is a anti-fuzzy normal subnearring of a nearring R. □

Theorem 2.3. *Let A and B be anti-fuzzy subnearring of the nearrings G and H, respectively. If A and B are anti-fuzzy normal subnearrings, then $A \times B$ is an anti-fuzzy normal subnearring of $G \times H$.*

Proof. Let A and B be anti-fuzzy normal subnearrings of the nearrings G and H respectively.

Clearly, $A \times B$ is an anti-fuzzy subnearrings of $G \times H$.

Let x_1 and x_2 be in G, y_1 and y_2 be in H.

Then (x_1, y_1) and (x_2, y_2) are in $G \times H$.

Now,

$$\begin{aligned}\mu_{A\times B}[(x_1,y_1)+(x_2,y_2)] &= \mu_{A\times B}(x_1+x_2, y_1+y_2)\\ &= \max\{\mu_A(x_1+x_2), \mu_B(y_1+y_2)\}\\ &= \max\{\mu_A(x_2+x_1), \mu_B(y_2+y_1)\}\\ &= \mu_{A\times B}(x_2+x_1, y_2+y_1)\\ &= \mu_{A\times B}[(x_2,y_2)+(x_1,y_1)].\end{aligned}$$

Therefore, $\mu_{A\times B}[(x_1, y_1) + (x_2, y_2)] = \mu_{A\times B}[(x_2, y_2) + (x_1, y_1)]$. And

$$\begin{aligned}\mu_{A\times B}[(x_1,y_1)(x_2,y_2)] &= \mu_{A\times B}(x_1x_2, y_1y_2)\\ &= \max\{\mu_A(x_1x_2), \mu_B(y_1y_2)\}\\ &= \max\{\mu_A(x_2x_1), \mu_B(y_2y_1)\}\\ &= \mu_{A\times B}(x_2x_1, y_2y_1)\\ &= \mu_{A\times B}[(x_2,y_2)(x_1,y_1)].\end{aligned}$$

Therefore, $\mu_{A\times B}[(x_1, y_1)(x_2, y_2)] = \mu_{A\times B}[(x_2, y_2)(x_1, y_1)]$.
Hence $A \times B$ is an anti-fuzzy normal subnearring of $G \times H$. □

Theorem 2.4. *Let A and B be fuzzy subsets of the nearrings R and H, respectively and $A \times B$ is an anti-fuzzy normal subnearring of $R \times H$. Then the following are true:*

(i) if $\mu_A(x) \geq \mu_B(e')$, then A is an anti-fuzzy normal subnearring of R.

(ii) if $\mu_B(x) \geq \mu_A(e)$, then B is an anti-fuzzy normal subnearring of H.

(iii) either A is an anti-fuzzy normal subnearring of R or B is an anti-fuzzy normal subnearring of H.

Proof. Let $A \times B$ be an anti-fuzzy normal subnearring of $R \times H$ and x, y in R and e' in H.
Then (x, e') and (y, e') are in $R \times H$.
Now, using the property that $\mu_A(x) \geq \mu_B(e')$, for all x in R.
Clearly A is an anti-fuzzy subnearring of R.
Now,

$$\begin{aligned}
\mu_A(x + y) &= \max\{\mu_A(x + y), \mu_B(e' + e')\} \\
&= \mu_{A\times B}((x + y), (e' + e')) \\
&= \mu_{A\times B}[(x, e') + (y, e')] \\
&= \mu_{A\times B}[(y, e') + (x, e')] \\
&= \mu_{A\times B}[(y + x), (e' + e')] \\
&= \max\{\mu_A(y + x), \mu_B(e' + e')\} \\
&= \mu_A(y + x).
\end{aligned}$$

Therefore,

$$\mu_A(x + y) = \mu_A(y + x),$$

for all x and y in R. Also,

$$\begin{aligned}\mu_A(xy) &= \max\{\mu_A(xy), \mu_B(e'e')\}\\ &= \mu_{A\times B}((xy),(e'e'))\\ &= \mu_{A\times B}[(x,e')(y,e')]\\ &= \mu_{A\times B}[(y,e')(x,e')]\\ &= \mu_{A\times B}[(yx),(e'e')]\\ &= \max\{\mu_A(yx), \mu_B(e'e')\}\\ &= \mu_A(yx).\end{aligned}$$

Therefore,

$$\mu_A(xy) = \mu_A(yx),$$

for all x and y in R.

Hence A is an anti-fuzzy normal subnearring of R.

Thus (i) is proved.

Now, using the property that $\mu_B(x) \geq \mu_A(e)$, for all x in H, let x and y in H and e in R.

Then (e, x) and (e, y) are in $R \times H$.

Clearly B is an anti-fuzzy subnearring of H.

Now,

$$\begin{aligned}\mu_B(x+y) &= \max\{\mu_B(x+y), \mu_A(e+e)\}\\ &= \max\{\mu_A(e+e), \mu_B(x+y)\}\\ &= \mu_{A\times B}((e+e),(x+y))\\ &= \mu_{A\times B}[(e,x)+(e,y)]\\ &= \mu_{A\times B}[(e,y)+(e,x)]\\ &= \mu_{A\times B}[(e+e),(y+x)]\\ &= \max\{\mu_A(e+e), \mu_B(y+x)\}\\ &= \mu_B(y+x).\end{aligned}$$

Therefore,

$$\mu_B(x+y) = \mu_B(y+x),$$

for all x and y in H. Also,

$$\begin{aligned}
\mu_B(xy) &= \max\{\mu_B(xy), \mu_A(ee)\} \\
&= \max\{\mu_A(ee), \mu_B(xy)\} \\
&= \mu_{A\times B}((ee), (xy)) \\
&= \mu_{A\times B}[(e, x)(e, y)] \\
&= \mu_{A\times B}[(e, y)(e, x)] \\
&= \mu_{A\times B}[(ee), (yx)] \\
&= \max\{\mu_A(ee), \mu_B(yx)\} \\
&= \mu_B(yx).
\end{aligned}$$

Therefore,

$$\mu_B(xy) = \mu_B(yx),$$

for all x and y in H.

Hence B is an anti-fuzzy normal subnearring of H.

Thus (ii) is proved.

(iii) is clear. □

3. Conclusion

In this paper, we have defined Anti-Fuzzy normal subnearring and proved its properties.

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PHYSICAL STRUCTURE STABILITY AND BIOINFORMATION OF 2-CHLORO BENZENESULFONAMIDE WITH DFT AND MOLECULAR DOCKING STUDIES

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Abstract

The molecular geometry of 2-chlorobenzenesulfonamide was optimized and characterized by UV-Vis, ^{1}H NMR ^{13}C NMR, FT-IR and FT-Raman spectral analysis. The vibrational frequencies were assigned theoretically. The charge transfer within the molecule is found by using NBO analysis and structure stability is discussed. By using MEP, the reactive sites of 2CBS is studied. The physicochemical property of title compound was investigated. Molecular docking studies was performed with two crystallographic protein structures (PDB ID: 6Y84 and 6LU7), found binding energy and active sites with SARS-CoV-2 M^{pro} virus.

Keywords: Benzenesulfonamide, NMR, MEP, NBO.

1. Introduction

In late 2019, Severe acute respiratory syndrome corona virus 2 (COVID-2019) caused clusters of Pneumonia like illness in Wuhan, China [1]. A total number of 1,051,635 persons in 208 countries were reported to be infected by SARS-CoV-2, which causes coronavirus disease 2019, a disease that had led to 75,000 deaths till April 4 and still increasing. The World Health Organization (WHO) announced that Covid-19 should be characterized as a pandemic on March 11, 2020 [2]. Many patients with mild disease who would not been tested in Italy at earlier. The Rapid testing strategy for SARS-CoV-2 was adopted by Republic of Korea in early identification led to who had mild or limited symptoms, results lower case-fatality rate in compared to Italy (1.0% vs 7.2%) [3]. The literature reveals, 25 drugs are in investigation for, to use Covid-19, with 10 in active

clinical trials. A combined lopinavirritonavir antiviral drug has controlled patients in China just a week after the virus had been identified [4]. In icelandic populations the percentage of males tested positive was greater than females (16.7% vs 11.0%) [5].

Benzenesulfonamide has wide spectrum in antimicrobial activity, veterinary practices and in pharmaceutical products which have bacterial, bioactive agents, artificial fibers, dyes and plasticizers [6]. Sulfonamide is one of the classical chemotypes associated with potent CA inhibiton [7 – 10]. The sulfonamide also known as synthons which interprets and used as protease inhibitor, antitumour, diuretic, antibacterial [11 – 15]. 4-amino-N-carbamimidoyl benzene sulfonamide synthesis and antimicrobial activity of schiff's was reported. [16]. Benzensulfonamide was combined with naphthoyl group, has important role in medicinal chemistry [17]. A benzenesulfonamide was synthesized and characterized by various spectroscopic and analytical techniques [18].

Hierarchical cluster analysis was examined for title related derivative the internal structure of the obtained data and the quantitative structureactivity relationship (QSAR) analysis with multiple linear regression (MLR) method was reported [19]. Several arylsulfonamides and their N-halo compounds are of great interest as they show pharmacological, fungicidal and herbicidal activities due to their oxidizing action in aqueous, partial aqueous and non aqueousmedia [20]. Selection of the right solvent and best operation conditions is pivotal to reach the optimal reaction yield of organic compounds synthesis. More importantly, the solvent and temperature are two crucial variables of crystallization for the purpose of purification, which would directly influence the crystal morphology, polymorph and other crystal performances [21 – 22]. The solubility of 2-chlorobenzenesulfonamide in 16 single pure solvents including methanol, ethanol, n-propanol, isopropanol, n-butanol, isobutanol, acetone, 2- butanone, 2-pentanone, cyclohexanone, cyclopentanone, ethyl acetate, methyl acetate, ethyl formate, acetonitrile and tetrahydrofuran was determined at temperature range from 273.15 to 324.65 K and atmospheric pressure [23]. Heterocyclic compounds bearing sulfonamide moiety possess diverse biological activities including antibacterial [24], a large group of 2- (benzylthio)-4-chloro-5-[(5-(substituted)-1,3,4-oxadiazol-2-yl)]benzenesulfonamides, and found that among them a series of (E)-2-(benzylthio)-4-chloro-5-(5-styryl-1,3,4-oxadiazol-2-yl)benzenesulfonamides display significant antitumour activity [25]. Analysis of the structureactivity relationship showed that the activity of compounds substituted with a chlorine atom in position 2 of benzenesulfonamide scaffold (R1 = Cl) is much more diverse and more dependent on the structure of Ar substituent than for compounds substituted with benzylthio in position 2 of benzenesulfonamide scaffold (R1 = SBn) which, however, show lower average activity. Analyzing the influence of different benzenesulfonamide scaffold, we have observed a more favorable effect of the sulfonamide group in the meta position to the oxadiazole ring, than in the para position, or for the total absence of sulfonamide moiety [26].

The presence of arylsulfonamide moiety at the p-position has been found to enhance the inhibitory potential peptidomimetic inhibitors of hepatitis C virus [27] we envisioned to combine these pharmacophores to synthesize novel S-benzyl-oxadiazole-benzene sulfonamides and S-alkylphthalimide-oxadiazole benzenesufon-amides. This article reports on the synthesis, bioassay screening against dengue protease (serotype-2), DENV2 NS2B/NS3pro, molecular docking analyses of these hybrids [28]. The studies reported below demonstrated that N-(4-cycloheptyl-4-oxobutyl)-4-methoxy-N-phenylbenzenesulfonamide (9), is a novel CaMKII inhibitor that displays anti-DENV and anti-ZIKV activity in both cell and animal studies [29]. Through literature search reveals there is no quatum chemical study has been carried out so far on the title compound. In present study we report, Geometrical structure properties, spectroscopic investigation, charge transfer analysis and biological of the 2-chloro benzenesulfonamide molecule.

2. Computational Methods

The Density functional theory calculation are performed using Gaussian09W software package [30] at B3LYP /6-311++G (d,p) basis set. The optimized structural parameters for the title molecule are studied by B3LYP Method. The MEP was stimulated using Gaussview 5.0 [31]. The vibrational assignment of the molecule was obtained using Veda4 Program [32]. The physicochemical properties of title compound were studied using online tool [33]. Molecular docking analysis was performed using autodock software package [34]. The P-L interaction was visualized using pymol graphical software interface [35].

3. Result and Discussion

3.1. Molecular Geometry

The molecular structure of 2chlorobenzenesulfonamide belongs to and in fig 1 optimized geometric molecular structure of 2CBS is visualized and the structural parameters are enlisted in table 1. The observed theoretical bond length parameters show consistent with respect to experimental values. The molecular formula and molecular weight of the compound is $C_6H_6ClNO_2S$ and 191.63 g/mol respectively. The title molecule comes under monoclinic crystal system, *cc* space group and with the cell dimension of a = 6.955 (1) Å, b = 14.848(3) Å c = 7.751(1) Å. The stimulated parameters of bond length, bond angle and dihedral angle are compared with experimental geometrical parameters [36]. The molecule contains six CC bonds, four CH bonds, two S=O and N-H bonds and each ClC, SC, SN bonds.

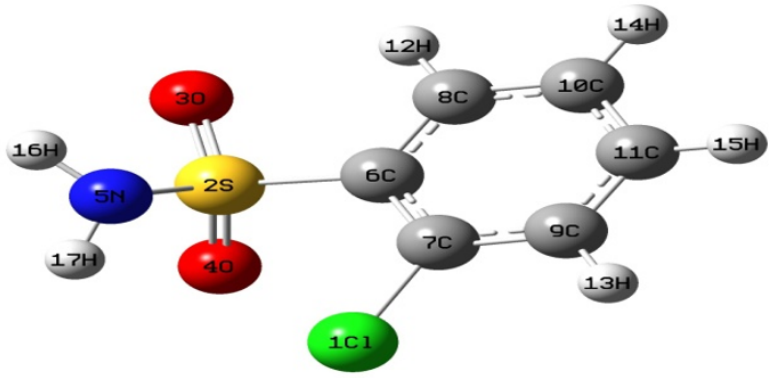

Figure 1: Molecular Structure of 2CBA

Table 1: Optimized Geometrical Parameter of 2CBS

Bond Length (Å)	B3LYP 6-311++ G (d,p)	Expt.	Bond Angle (o)	B3LYP 6-311++ G (d,p)	Expt.	Dihedral Angle (o)	B3LYP 6-311++ G (d,p)	Expt.
Cl1-C7	1.7517	1.737 (3)	O3-S2-O4	121.4206	118.92 (13)	O3-S2-N5-H16	14.4564	–
S2-O3	1.4607	1.429 (2)	O3-S2-N5	106.2137	106.32 (13)	O3-S2-N5-H17	140.4514	–
S2-O4	1.457	1.4275 (19)	O3-S2-C6	106.5891	105.88 (12)	O4-S2-N5-H16	-118.2565	–
S2-N5	1.6837	1.600 (2)	O4-S2-N5	109.436	107.32 (12)	O4-S2-N5-H17	7.7385	–
S2-C6	1.8101	1.784 (2)	O4-S2-C6	108.4978	108.31 (12)	C6-S2-N5-H16	126.3887	–
N5-H16	1.0145	0.857 (19)	N5-S2-C6	103.1859	109.91 (11)	C6-S2-N5-H17	-107.6163	–
N5-H17	1.0142	0.835 (18)	S2-N5-H16	109.9533	116 (2)	O3-S2-C6-C7	173.7676	178.5 (2)
C6-C7	1.3985	1.384 (4)	S2-N5-H17	111.5925	113 (2)	O3-S2-C6-C8	-8.3548	-3.7 (2)
C6-C8	1.3947	1.385 (4)	H16-N5-H17	112.8354	114 (3)	O4-S2-C6-C7	-53.9134	-52.9 (2)
C7-C9	1.392	1.389 (4)	S2-C6-C7	123.6371	–	O4-S2-C6-C8	123.9642	124.8 (2)
C8-C10	1.3913	1.393 (4)	S2-C6-C8	116.5745	117.2 (2)	N5-S2-C6-C7	62.1116	64.0 (2)
C8-H12	1.0823	0.93	C7-C6-C8	119.7546	119.8 (2)	N5-S2-C6-C8	-120.0108	-118.19 (19)
C9-C11	1.3922	1.376 (5)	Cl1-C7-C6	122.2701	–	S2-C6-C7-Cl1	-2.8583	-2.5 (3)
C9-H13	1.0824	0.93	Cl1-C7-C9	117.7698	123.0 (2)	S2-C6-C7-C9	177.8621	178.4 (2)
C10-C11	1.392	1.366 (5)	C6-C7-C9	119.9564	–	C8-C6-C7-Cl1	179.3282	179.77 (19)
C10-H14	1.0832	0.93	C6-C8-C10	120.2464	119.8 (3)	C8-C6-C7-C9	0.0486	0.7 (4)
C11-H15	1.0838	0.93	C6-C8-H12	118.561	120.1	S2-C6-C8-C10	-177.7432	–

3.2. Vibrational Assignments

Vibrational spectroscopy is much important tool to evaluate the functional groups of organic compounds [37]. The theoretically observed FT-IR, FT-Raman spectrum is

shown in Fig 2 and 3. The molecule consists of 17 atoms with 45 vibrational modes of frequency. The potential energy distributions were calculated. The stimulated frequencies, IR intensity, Raman activity and PED with stretching bending and torsional vibrations of 2CBS are listed out in Table 2.

Table 2: Vibrational Assignment of 2CBS

MODES	UNSCLAED	SCALED	IR INTENSITIES	RAMAN INTENSITIES	ASSIGNMENTS (PED)
45	3627	3485	2	0	–
44	3516	3379	0	0	γNH(100)
43	3209	3084	1	1	–
42	3203	3078	1	1	γCH(12)
41	3193	3068	2	4	γCH(100)
40	3178	3054	3	3	γCH(86)
39	1617	1554	12	2	–
38	1610	1547	9	8	γCC(12)
37	1580	1518	7	9	–
36	1484	1427	24	1	–
35	1463	1406	26	0	γCC(24)
34	1326	1274	3	1	γCC(30)
33	1314	1262	0	9	γSO(44)+γCC(26)
32	1280	1230	3	5	β HCC(61)+γCC(30)
31	1188	1142	28	2	β HCC(66)
30	1153	1108	15	0	γCC(44)+β HCC(26)
29	1133	1089	5	4	γSO(29)+β HCC(10)
28	1106	1063	1	0	–
27	1088	1045	14	0	γCC(10)β HNS(66)+γSO(22)
26	1057	1015	0	0	γCC(75)
25	1042	1001	0	14	β CCC(27)
24	1004	965	0	5	γSO(42)
23	976	938	41	1	τHCCC(66)
22	882	848	15	0	τHCCC(100)
21	849	816	3	0	τHNSC(25)
20	771	741	1	14	τHCCC(94)
19	744	715	1	8	β CCC(12)
18	717	689	44	1	τCCCC(18)
17	668	642	23	0	β CCC(71)
16	614	590	4	1	γSN(23)+τHNSC(46)
15	554	533	1	1	–

14	543	522	2	0	τCCCC(15)
13	486	467	2	0	β OSO(21)
12	468	450	1	0	OUTONCS(13)
11	433	416	1	0	γClC(18)+β OSO(22)
10	415	399	1	0	γClC(12)+β OSO(15)
9	376	361	1	1	OUTONOS(15) + τHNSC(10)
8	306	294	1	1	τCCCC(13) + OUTClCCC(11) + OUTONCS(17) +βOSO(10)
7	278	268	3	1	γSC(32)+β NSC(14)
6	266	255	2	0	β ClCC(34) + βNSC(10)+ OUTONCS(21)
5	181	174	2	0	βOSN(10) +τCCCC(23) +OUTClCCC(18) +τHNSC(24)
4	175	169	0	0	OUTClCCC(15) +τHNSC(15)
3	151	146	1	0	β SCC(38)+β OSN(10)+ β ClCC(11)
2	105	101	0	0	OUTSCCC(27) +τCCCC(32)
1	65	62	0	0	τNSCC(68) +OUTSCCC(23)

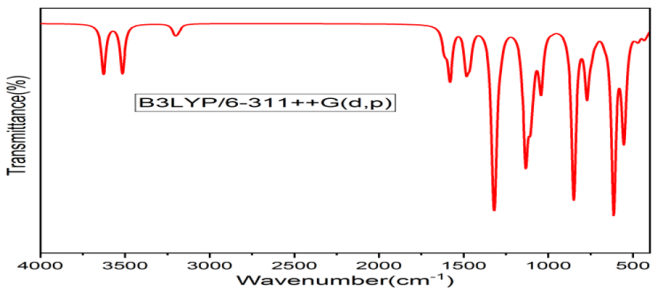

Figure 2: FT-IR Spectrum of 2CBS

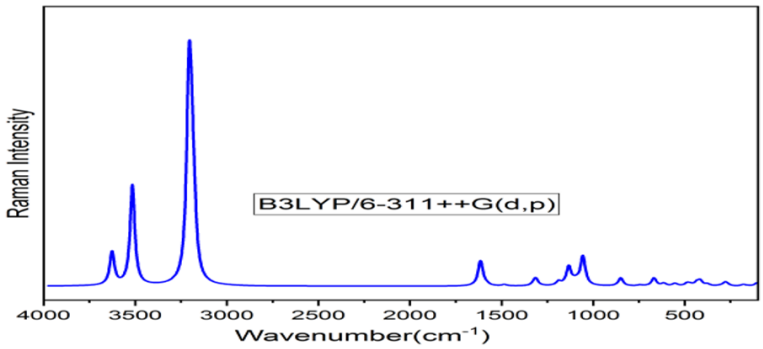

Figure 3: FT-Raman Spectrum of 2CBS

3.2.1 NH Vibration

The N-H stretching vibration appears strongly in the range of 35003300 cm^{-1}. [38]. The NH vibrations observed frequency is 3485, 3379 and 3084 cm^{-1} with 100% PED.

3.2.2 CH Vibration

The heteroaromatic organic compounds and its derivatives commonly exhibit multiple peaks in the region 3100-3000 cm^{-1} [39]. The observed 3078, 3068 and 3054 cm^{-1}. The 3068cm^{-1} frequency shows 100% CH stretching vibration.

3.2.3 CC Vibration

For aromatic and hetero aromatic compounds CC vibrations are assigned to the range 1650-1400 cm^{-1} [40]. The expected ring stretching vibrations are in the range of 1300-1000 cm^{-1} [41]. The calculated CC vibrations are observed at 1554, 1547, 1518, 1427, 1406 and 1274 cm^{-1}. The ring vibrations are observed at 1015cm^{-1} with 75% of PED.

3.2.4 S=O Vibrations

The S=O strong stretching vibration is observed at for sulfonamide derivative was at 1370-1335 [42]. The calculated frequency is 1262 and 965 cm^{-1}.

3.2.5 C-Cl Vibrations

The vibrations belonging to the bond between the ring and chlorine atoms are worth to discuss here since mixing of vibrations is possible due to the lowering of the molecular symmetry and the presence of heavy atoms on the periphery of the molecule. Mooney

assigned vibrations of C-Cl, Br and I in the wave number range of 1129-480 cm^{-1} [43-44]. The calculate chlorine carbon bond vibration is at 450 with 18% of maximum PED.

3.3. Molecular Electrostatic Potential

The space around a molecule is created by electrostatic potential V(r), its nuclei and electrons treated as static distributions of charge is a very useful property for predicting and analyzing reactive molecular behavior. It is rigorously defined and can be determined experimentally as well as computationally. The molecular electrostatic potential is related to electron density and a very useful descriptor for determining sites for electrophilic attack and nucleophilic reactions as well as hydrogen-bonding interactions [45-46]. The ESP map enable to study about the 3D charge distribution for the molecule [47].

To predict electrophilic and nucleophilic reactive sites of 2CBS using B3LYP level optimized geometry with the basis set 6-311++G(d,p) was calculated and displayed in Fig. 4. The positive electrostatic potential is blue colour in region around to the hydrogen atoms H16 and H17 is repulsion of the proton by the atomic nuclei, nucleophilic region. The negative electrostatic potential red in colour around the oxygen atoms O3 and O4 is electrophilic region of the molecule.

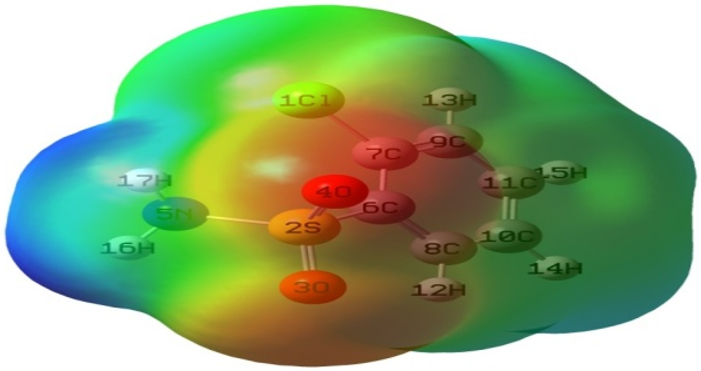

Figure 4: ESP Map of 2CBS

3.4. NMR Studies

The NMR spectrum is used to identify the shielding and de-shielding effect in an atom of the molecules. The stimulated chemical shift values for carbon (13C) and proton (1H) NMR of the title compound spectrum was shown in Fig. 5. The theoretical 13C and 1H chemical shifts are calculated from B3LYP/6-311++G (d,p) using GIAO method [49]. The GIAO method is important method to calculate isotropic nuclear magnetic shielding tensors [49]. In carbon atoms C10 with maximum of 20 ppm and in hydrogen atoms the maximum value is H16 with 27 ppm.

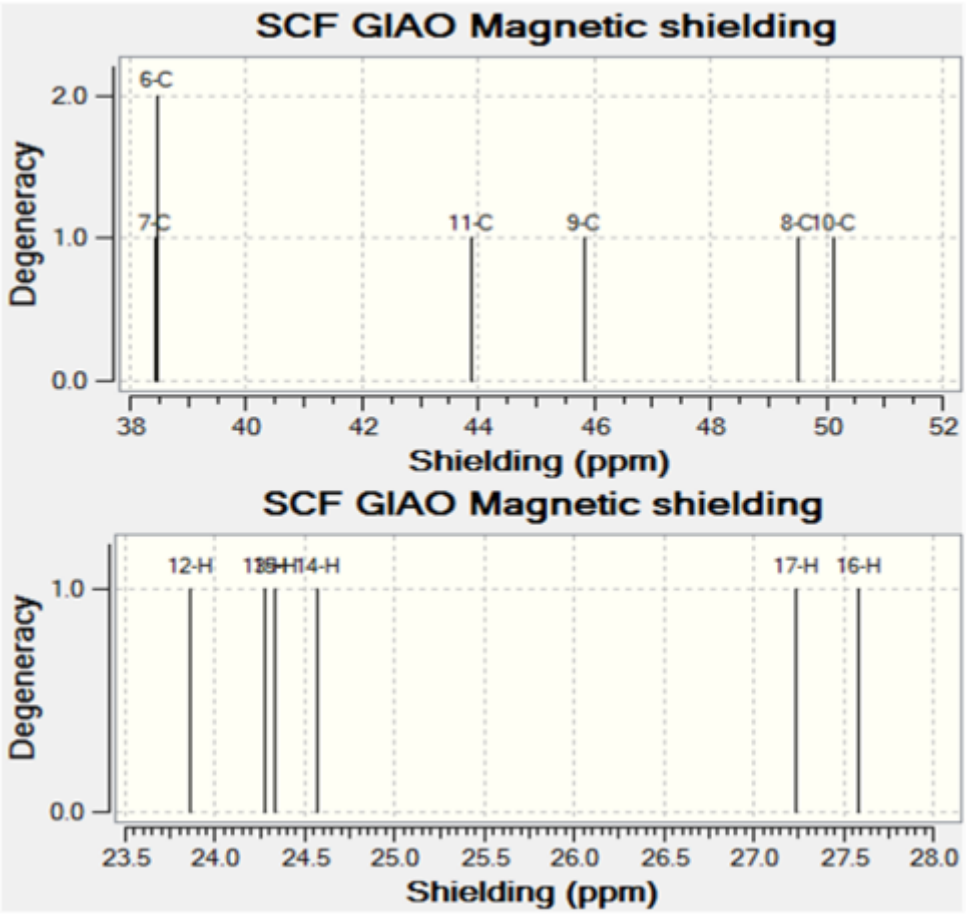

Figure 5: ^{13}C and ^{1}H NMR Spectrum of 2CBS

3.5. UV Absorption Spectra

On the basis of fully optimized ground-state structure, TD-DFT/B3LYP/6-311++G (d,p) calculations have been used to determine the low-lying excited states of MNMB. The UVVis absorption spectrum of the sample in ethyl acetate is shown in Fig. 6. The calculated results involving the vertical excitation energies, oscillator strength (f) and wavelength are carried out [50]. The literature reveals that, the solubility of mole fraction in different alcohols ranked as methanol > ethanol > n-propanol > isopropanol > n-butanol > isobutanol, which is in accordance with the dielectric constant and Hildebrand solubility parameter [51]. According to FrankCondon principle, the maximum absorption peak (kmax) corresponds in an UVVis spectrum to vertical excitation. TD-DFT/B3LYP/6-311++G (d,p) absorption spectra of methanol predicts electronic transition at 231 nm with an oscillator strength f = 0.0994.

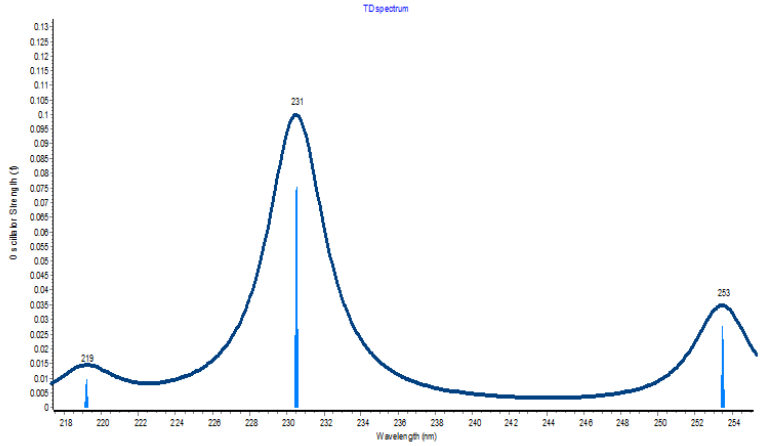

Figure 6: UV-Vis Spectrum of 2CBS with Methanol

3.6. NBO Analysis

The natural Lewis structure picture of Φ is analyzed using NBO all orbital details are mathematically chosen to include the highest possible percentage of the ED. Interaction between filled and virtual orbital spaces information is correctly explained and could enhance the analysis of intra and intermolecular interactions [52]. The second order fock matrix was carried to evaluate donor (*i*) and accecptor (*j*) and stabilization energy E(2). The π^* C6-C7 to π^* C9-C11 interaction gives strong stabilization energy and strengths the structure stability. The interaction between LP(3) O4 and σ^* S2-N5 increases the ED in anti-bonding orbital's weakens the respective bonds and this charge transfer interaction contributes the title molecule towards bio activeness.

Table 3: Natural Bond Orbital Analysis

Donor	NBO(i)	Acceptor	NBO(j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
π^*	C6-C7	π^*	C9-C11	111.02	0.03	0.083
π^*	C6-C7	π^*	C8-C10	103.2	0.03	0.082
π	C9-C11	π^*	C6-C7	23.92	0.25	0.071
π	C8-C10	π^*	C9-C11	21.33	0.28	0.07
π	C8-C10	π^*	C6-C7	20.7	0.25	0.066
π	C6-C7	π^*	C8-C10	19.41	0.31	0.07
π	C9-C11	π^*	C8-C10	18.38	0.28	0.065
π	C6-C7	π^*	C9-C11	15.87	0.31	0.063
π^*	C6-C7	σ^*	S2-N5	7.05	0.11	0.042
σ	C6-C8	σ^*	C6-C7	5.73	1.27	0.076
σ	C6-C7	σ^*	C6-C8	5.07	1.3	0.073
σ	C6-C8	σ^*	Cl1-C7	4.83	0.89	0.059

σ	C7-C9	σ^*	C6-C7	4.82	1.27	0.07
σ	C9-C11	σ^*	Cl1-C7	4.53	0.87	0.056
σ	C9-H13	σ^*	C6-C7	4.42	1.07	0.062
π	C6-C7	σ^*	S2-N5	4.33	0.4	0.037
σ	C8-H12	σ^*	C6-C7	4.31	1.07	0.061
LP(3)	O4	σ^*	S2-N5	19.74	0.39	0.079
LP(3)	O3	σ^*	S2-N5	18.19	0.39	0.076
LP(2)	O4	σ^*	S2-C6	17.41	0.47	0.081
LP(2)	O3	σ^*	S2-C6	17.2	0.47	0.08
LP(3)	Cl1	π^*	C6-C7	16.61	0.3	0.07
LP(3)	O3	σ^*	S2-O4	16.6	0.59	0.09
LP(3)	O4	σ^*	S2-O3	15.81	0.58	0.087
LP(2)	O3	σ^*	S2-N5	8.91	0.4	0.054
LP(2)	O4	σ^*	S2-N5	7.71	0.39	0.05
LP(2)	Cl1	σ^*	C6-C7	5.61	0.85	0.062
LP(2)	O4	σ^*	S2-O3	5.11	0.58	0.049
LP(2)	O3	σ^*	S2-O4	4.26	0.59	0.045

4. Physicochemical Properties

The physicochemical properties were used to predict aquatic bioavailability and toxicity within the molecule [53]. A physicochemical range on each axis was defined by descriptors adapted [54-55]. The topological polar surface area (TPSA) is calculated using the fragmental technique [56]. The calculated parameters are enlisted in Table 5. The topolocial polar surface area is calculated at 68.54Å.

Table 4: Physicochemical Properties of 2CBS

Physicochemical Properties	
No. heavy atoms	11
No. arom. heavy atoms	6
Fraction Csp3	0
No. rotatable bonds	1
No. H-bond acceptors	3
Num. H-bond donors	1
Molar Refractivity	42.45
TPSA	68.54^2

4.1. Molecular Docking

Molecular docking plays an important role in drug discovery to predict the protein ligand interaction, molecular mechanism and binding site [57]. The solvent and water in protein were removed using pymol graphical interface [58] and docking was performed using auto dock program [59]. In order the title molecule is carried out to predict the L-P interactions. The docking simulations were carried out for two SARS-CoV-2 Proteins. The title molecule was subjected to study the interactions with crystal structure PDB ID; 6Y84 and 6LU7. Proteins were downloaded from RSCB database [60]. The docking parameters are enlisted in Table 8 includes bonded residues, bonded distance, binding energy and RMSD references. The binding energy was calculated for 6Y84 protein is 6.52 kcal/mol and 6LU7 protein is 5.33 kcal/mol. The docked figures with bonded residues are visualized in 9 & 10. The title molecule shows good binding affinity towards both the antiviral proteins. The title molecule might be potential drug for SARS CoV-2 antiviral protein.

Table 5: Docking and Hydrogen Bond Parameters

PDB	Bonded Residue	Hydrogen Bond Interaction P....L	No. of hydrogen bond	Bonded Distance (Å)	Binding energy (kcal/mol)	RMSD ID
6Y84	Arg'4	O....H	3	2.1	-6.52	9.39
	LYS'5	O....H		2.3		
	PHE'3	H....O		1.9		
6LU7	ARG'217	O....H	4	2.3	-5.33	55.66
	THR'257	H....O		3.3		
	VAL'212	H....O		1.9		
	THR'304	H....O		2		

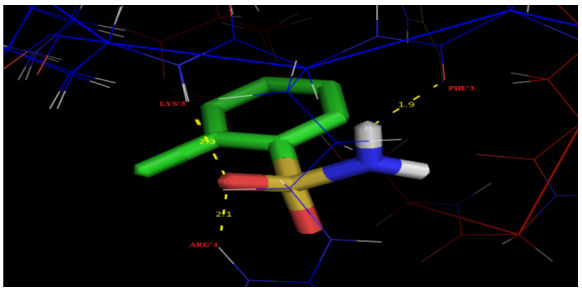

Figure 7: Docked Image of 6Y84 COVID Protein with 2BCS

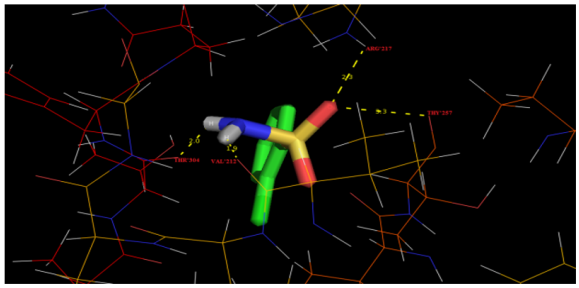

Figure 8: Docked Image of 6LU7 COVID Protein 2CBS

5. Conclusion

In present work, we have characterized 2 chlorobenzene sulfonamide using UV-Vis, FT-Raman, FT-IR and NMR spectral analysis. The optimized geometry is tabulated and compared with XRD data. DFT B3LYP method at 6-311++G (d,p) was used to perform in entire work. Stimulated vibrational modes were analysed using PED. The NBO is performed to study the intra molecular interaction within the molecule. The ESP map is visualized with electrophilic and nucleophic region of 2CBS. The physicochemical properties of the title molecule have been reported. The binding sites of SARS CoV-2 protein is found with the title ligand. The result reveals the 2CBS molecule has antiviral activity against SARS CoV-2 virus and it was predicted as a potential inhibitor COVID-19 disease.

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SYNTHESIS AND CHARACTERIZATION OF IRON OXIDE NANOPARTICLES ON AGAR-AGAR AND PECTIN TEMPLATES

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Abstract

Magnetite (Fe_3O_4) nanomaterial has gained much attention in the biomedical field. synthesizing solubilized magnetite nanoparticles is difficult due to aggregation and poor biocompatibility. Here we report the synthesis of Nano-composites comprised of magnetite (Fe_3O_4) nanoparticles in a pectin and Agar - Agar by the co-precipitation method. X Ray diffraction (XRD) of the prepared sample revealed the crystalline character and size of the magnetite nanoparticles were about 200nm. FT-IR results confirm the formation of Fe_3O_4 nanoparticles in biopolymer matrix. Analysis of the absorption coefficient has been carried out and the nature of transitions and the optical band gap Eg are determined.

Keywords: Bio Molecules, Co-precipitation, Agar - Agar, Pectin.

1. Introduction

Magnetic nanoparticles are of great interest both for fundamental research and emerging applications. Nanoparticles are capable to reach the sub cellular level as most of the apertures, openings, and gates at cellular or sub cellular levels are of nanometer size [1, 2]. Materials used for magnetic biomedical applications should be super paramagnetic, non-toxic and biocompatible. These super paramagnetic materials are of interest because they do not retain any magnetism after removal of the magnetic field; this fact implies that non- or low-coercive forces exist, preventing magnetic dipolar interactions between particles and, eventually, their aggregation [3 – 5]. Magnetite (Fe_3O_4) is the most widely used iron oxide nano-particles with diverse applications. Bare magnetite nanoparticles on account of their large surface area /volume ratio tend to agglomerate. To prevent agglomeration, a variety of polymeric coatings have been

applied to nanoparticles. Among the polymeric capping agents, bio-polymers are of special interest due to their biocompatibility and biodegradability. Coating is essential because it reduces aggregation of nanoparticles thereby improving their dispersibility, colloidal stability and protects their surface [6 – 8].

Co-precipitation and thermal decomposition methods have been the two most widely used methods for the synthesis of iron oxide nanoparticles. The co-precipitation method is simple, cost-effective and favored for biological applications due to its processing temperature and environmental friendly conditions.

In the present study, the biopolymers agar agar and pectin was used because of their potential use in biomedical applications. The biological function of agar is offering a flexible structure to algae, helping them to withstand the varying forces of currents and wave motions [9, 10]. Chemically, it is mainly composed of alternating β-(1-3)-d-galactose and α-(1-4)-3,6-anhydrol-galactose repeating units [9]. agars from Gelidium contain much lower amount of sulphate in the molecule when compared to those from Gracilaria, and thus providing stronger gels [11 – 12].

Pectin is a group of complex polysaccharides that contain 1, 4-linked α-D-galacturonic acid [13 – 15]. Pectin has a very complex structure that depends on both its source and the extraction process [16 – 18]. Pectin is biodegradable, biocompatible and is reported to be bioactive [19]. The presence of hydroxyl ($-$OH) functional group in pectin enhances its chemical properties and COOH groups which permit direct bonding to Fe_3O_4. A coating of pectin on the nanoparticles reduces the interactions of the electrostatic particles and as a result significantly augments the stability of the diffusion colloid [20].

The presence of agar and pectin coating was confirmed by Fourier transform infrared spectroscopy (FTIR) The morphology, crystal grain sizes and structure of Fe_3O_4 with agar agar and pectin were determined by X-ray diffraction (XRD). Based on our results, we discuss its potential uses.

2. Experimental

2.1. Materials

All chemical reagents were analytical grade and used without further purification. $FeCl_3$.$6H_2O$, $FeCl_2$ $4H_2O$, $FeSo_4$ $7H_2O$, Agar - Agar, pectin, deionized water, aqueous ammonia and ethanol were purchased from M/s JAYSUN Chemicals, India. The pH meter was employed to control the pH of the solution. The Laboratory Oven was used to dry and the washed samples.

2.2. Synthesis of Fe_3O_4

Iron oxide (Fe_3O_4) were synthesized using co precipitate method by dissolving appropriate amount of ferrous chloride (Fe Cl_2 $4H_2O$) and ferric chloride (Fe Cl_3 $6H_2O$)

in deionized water. The mixture was mixed slowly in aqueous ammonia solution with vigorous stirring for 30 minutes. The pH of the solution was maintained in between 11 and 12 using concentrated ammonium hydroxide solution. The resultant mixture was centrifuged for 10 minutes to obtain the nanoparticles. The obtained precipitate was washed three times with distilled water and tetra hydrofurane (THF) and then dried in the air for a period of 12 hrs.

2.3. Synthesis of Agar - Agar

2.5g of agar agar was dissolved in 100 ml of de-ionized water in order to prepare iron oxide with the agar -agar template. $FeSo_4.7H_2O$ was added to assess the volume of the template solutions so that the polysaccharide and Fe ratio ranged from 1:4. The resulting solution was stirred for 30 minutes. The template-iron mixed solution was annealed at a temperature of 800°C with the heating rate of 5°C/min for 120 minutes. The temperature was allowed to fall at the rate of 10°C/ min to room temperature.

2.4. Synthesis of Pectin

2.5g of pectin was dissolved in 100 ml of water in order to prepare iron oxide with a pectin template. $FeSo_4$ $7H_2O$ was added to know the volume of the template solutions such that the polysaccharide Fe ratio 1:4. The resulting solution was stirred for 30 minutes. The template-iron mixed solution was treated at 800°C and kept for 120 minutes at that temperature, after which it was cooled at a rate of 10°C/minutes to room temperature.

2.5. Characterization

The synthesized material was subjected to various characterizations. Powder X-ray diffraction (XRD) patterns were recorded by a Bruker Model: D8 Advance diffractometer with CuK radiation (1.54Å) operating at 40 kV and 30mA.The IR spectra were obtained using a Perkin Elmer IR Spectrometer instrument at room temperature in the 4000400cm^{-1} range. The UV-Vis spectrum of Fe_3O_4 -NPs was determined using UV -Visible Spectrophotometer (UV-1800).

3. Results and Discussion

The iron oxide Fe_3O_4 was synthesised with and without pectin and agar - agar polysaccharide templates.

3.1. FT IR Analysis

The iron oxide Fe_3O_4 templates pectin and agar agar were subjected to FT-IR analysis with and without bio-polymers. The Fourier transform infrared of iron oxide absorption

spectrum with and without bio-polymers is given as Fig. (1) provides a range of reports on Pectin FT-IR absorption studies showing characteristic peaks at 556-642, 1467-1095, 1707-1606 and 3525-3786 cm^{-1}. The frequency number range of 1104 cm^{-1} present in (compounds containing nitrogen oxygen bond) C form of bond of stretching mode of vibration is found in pectin templates. The frequency number range of 1102 cm^{-1} present in (compounds containing nitrogen oxygen bond) C form of bond of stretching mode of vibration is found in Iron oxide with pectin template.The frequency number range of 2366cm^{-1} present in Ammonia compounds containing of NH_3+ bond of stretching mode of vibration is found in pectin template the frequency number range of 2379cm^{-1} present in Ammonia compounds containing of NH_3+ bond of stretching mode of vibration is found in Iron oxide with pectin templates. The frequency number range of 2925cm^{-1} present in Ammonia compounds containing of -CH_3 bond of stretching mode of vibration is found in pectin template The frequency number range of 2919cm^{-1} present in Ammonia compounds containing of -CH_3 bond of stretching mode of vibration is found in Iron oxide with pectin templates.

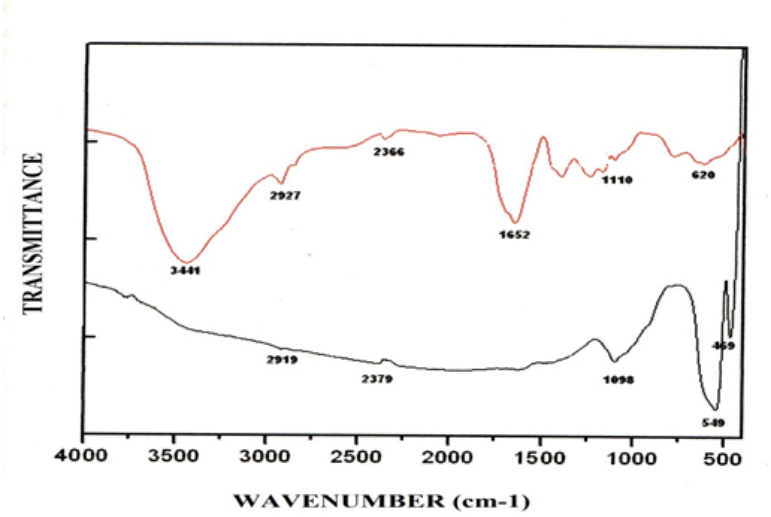

Figure 1: FT IR Spectrum of Pectin and Iron Oxide with Pectin Template

The Fourier transform infrared of iron oxide absorption spectrum with and without bio-polymers is given as Fig. (2 & 3) provides the number of reports on the FT-IR absorption studies of Agar Agar showing characteristic peaks at 556-560, 1131-1383, 1411-1534, 1626-1700 and 3414-3423cm^{-1}.The reported characteristic peak of Fe-O group of iron oxide located In the 560cm^{-1} in our study the peak of Fe-O group of iron oxide located at 560.50 cm^{-1} for iron oxide without templates in the synthesis of iron oxide with Agar-Agar templates the characteristic peak reduced to 556.54cm^{-1}. When the iron oxide (Fe_3O_4), the peaks of stretching of NH_2 at 3423.25cm^{-1} is shifted to 3414.27 cm^{-1} for iron oxide with agar-agar templates. When the iron oxide (Fe_3O_4),

the peaks of stretching at 1629.23 cm^{-1} is shifted to 1626.23 cm^{-1} for iron oxide with agar-agar templates.

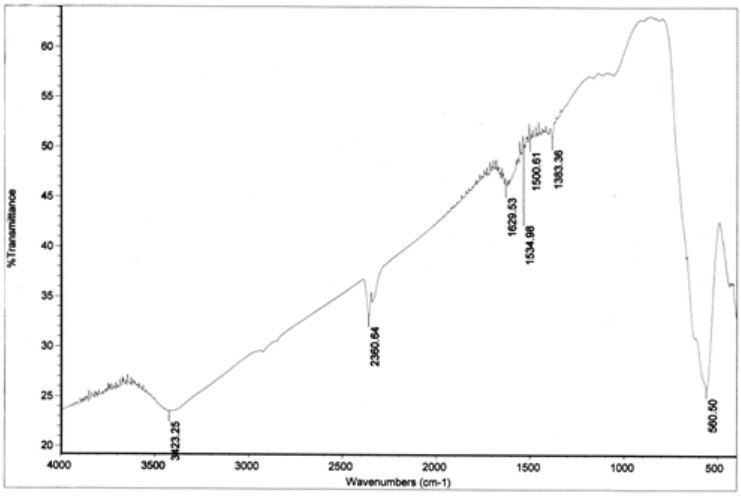

Figure 2: FT-IR Spectrum of Iron Oxide

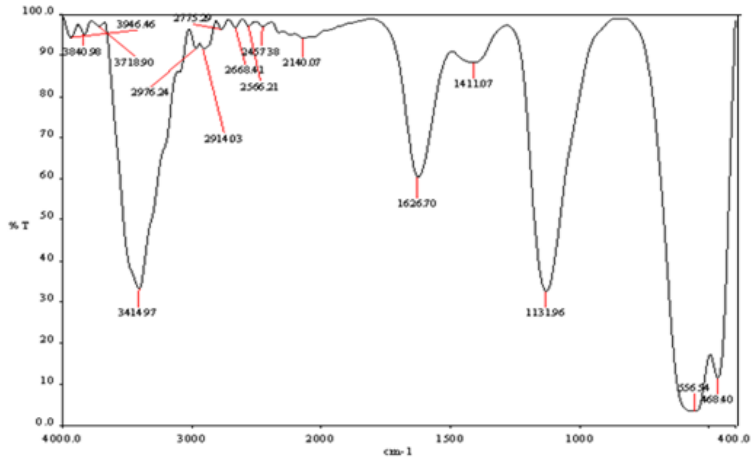

Figure 3: FT IR Spectrum of Iron Oxide with Agar - Agar Templates

3.2. XRD Analysis

An XRD analysis was performed on the iron oxide Fe_3O_4 with pectin and agar agar biopolymer templates.

As can be seen in Fig. 4 and 5. The XRD patterns of agar - agar and pectin did not vary clearly between them. The powder XRD patterns also showed different peaks with values of approximately 33.13°, 35.62°, 49.44°, 54.08° and 63. 51° for agar agar, for pectin, the $2\theta^{\circ}$ values are approximately 33.04°, 35.61°, 49.46°, 54.02° and 64.04° respectively. These peak locations and relative peak intensities corresponded to the Fe_3O_4 peaks, so it was determined that pectin and agar - agar magnetic Fe_3O_4 nano particles were successfully manufactured. Agar - Agar diffraction peaks showed wider FWHM than pectin (full width at half-maximum). The crystalline sizes could be determined from FWHM using the formula of scherrer expressed as D = 0.89 / ($\beta \cos \theta$), where β is the wavelength of the XRD peaks, β is FWHM and x is the angle of diffraction. The agar - agar Fe_3O_4 nano particles were clearly smaller than pectin. Since no apparent polysaccharide crystallinity was observed, the polysaccharide portion was in the amorphous phase, which could be the Fe_3O_4 polysaccharide hydrophilicity.

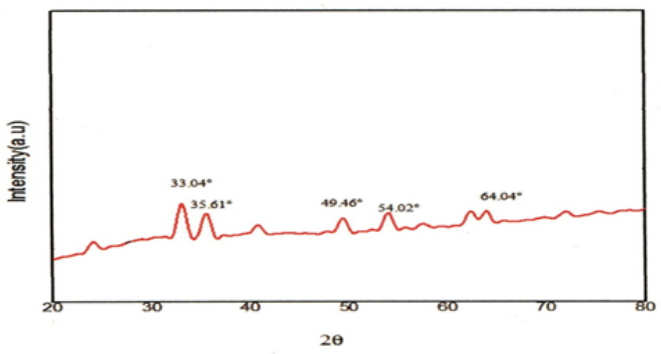

Figure 4: XRD Spectrum of Pectin with Fe_3O_4

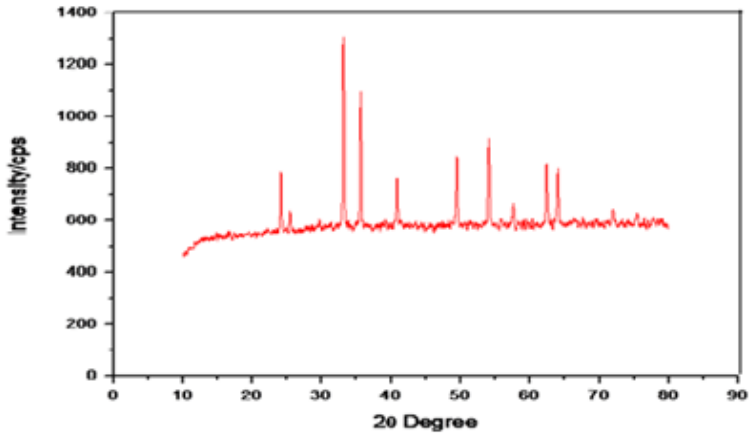

Figure 5: XRD Spectrum of Agar Agar with Fe_3O_4

3.3. UV Visible and Micro Structural Analysis

UV analysis was performed on the Biopolymer template pectin and agar agar with iron oxide without iron oxide. For biopolymer templates like pectin and agar agar with iron oxide without iron oxide, the spectral distributions of transmittance (T) dates are analysed in the spectral area (300-800 nm).

Analysis of the absorption coefficient has been carried out to determine the existence of the transitions involved and to obtain the distance in the optical band Eg involves plotting $(\alpha h\nu)^2$ against $h\nu$. Figure (8 & 9) shows that linear functions are the plots of $(\alpha h\nu)^2$ vs $h\nu$. This linearity indicates the presence of transitions permitted directly. The linear dependency extrapolation of both abscissa relationships gives the corresponding bandwidth Eg. The value of the optical energy gap with pectin (1.00 eV), agar agar (0.50 eV) models obtained for iron oxide.

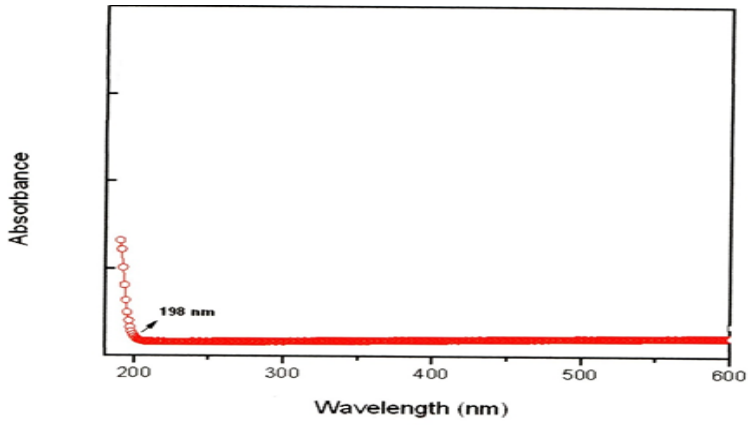

Figure 6: UV Spectrum of Pectin

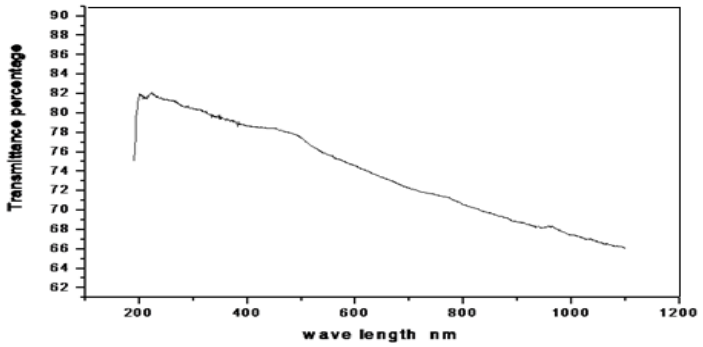

Figure 7: UV Spectrum of Agar - Agar

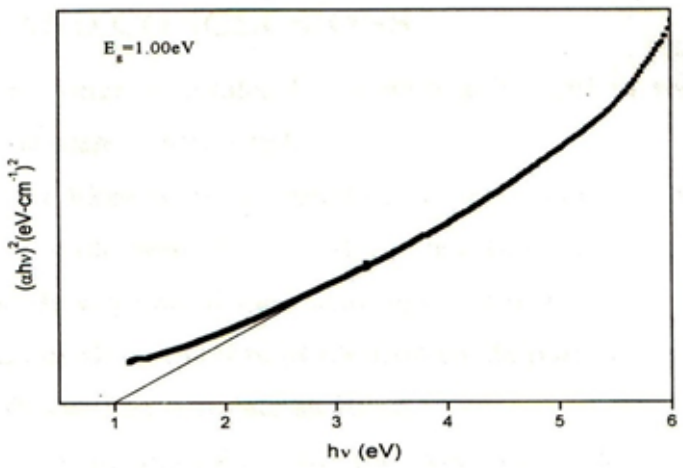

Figure 8: Plots of $(\alpha h\nu)^2$ versus hν Direct Transition of Pectin / Fe_3O_4

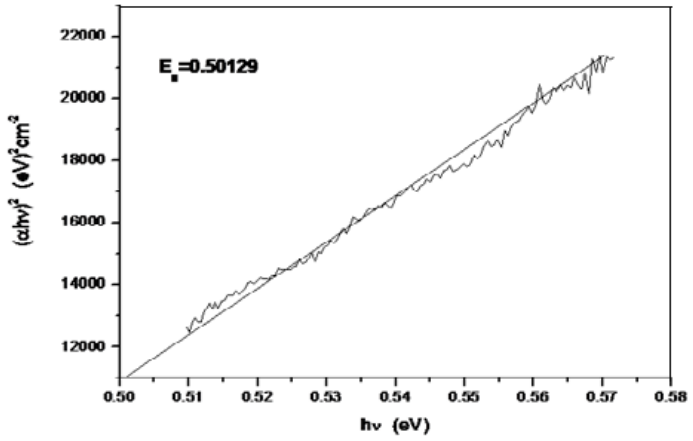

Figure 9: Plots of $(\alpha h\nu)^2$ versus hν direct transition of Agar - agar / Fe_3O_4

4. Summary and Conclusion

In this work, we report on the use of agar-agar and pectin as a biocompatible matrix to synthesize Fe_3O_4 magnetic nanoparticles, with the resulting particles encapsulated in agar-agar and pectin. FTIR of iron oxide with and without biopolymer templates such as pectin and agar - agar confirmed the formation of template free iron oxide. The XRD peaks shows the crystalline structure of material and indicate the absence of polysaccharide templates. The crystalline size of agar-agar template iron oxide is clearly smaller than the pectin template iron oxide. The UV-Visible study demonstrates the presence of direct permissible transitions and the values of the band gap are measured between semiconductor ranges.

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HF AND DFT STUDIES ON N-ETHYL-P-TOLUENE SULFONAMIDE

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Abstract

The structural properties of N-ethyl-P-toluenesulfonamide have been investigated by using ab initio-HF and DFT-B3LYP method with 6-311++G(d,p) basis sets. The absorption wavelength of UV-Vis spectra is calculated by TD-DFT method. The ^{1}H and ^{13}C NMR chemical shifts values are calculated for the title compound by using same level theory. HOMO and LUMO orbitals energy have been calculated. The stability and charge transfer of the molecule has been analyzed using natural NBO analysis. MEPS, Mulliken charges, IR and Raman intensities were calculated. Furthermore, protein ligand interaction study with SARS-CoV-2 virus has also been reported.

Keywords: SULFONAMIDE, NMR, Mulliken Charges, SARS-CoV-2.

1. Introduction

The title compound N-ethyl-P-toluenesulfonamide is a Sulfonamide derivative. Sulfonamide derivative is a heterocyclic compound, which is widely used in wide range of biological properties including antimicrobial, antibacterial, antitumor, antiinflammatory and analgesic activities [1 – 4]. Recent study indicated that cyclic sulfonamide derivatives are a promising new template for the development of anti-SARS-CoV-2 agents [5]. The two sulfonamide compounds are against HSV-1 virus, 7e and 13a, were evaluated for their inhibitory activity against USP7. Molecular Operating Environment were used to identify the interactions between 7e and 13a compounds using docking studies and the active site of the USP7 enzyme [6]. Abundance level of sulfonamide antibiotic resistance genes (ARGs) is reported in earlier studies [7]. Sulfonamide demonstrates great ability in the transition metal complexes of benzene sulfonamide and are synthesized with metals such as

Co(II), Mn(II), Cr(III),Fe(II), Fe(III), Ni(II), Zn(II) and Cu(II) [8]. $FeCl_2$ / K_2CO_3 catalyst system has developed for the N-alkylation of sulfonamides with benzylic alcohols. Characterization and crystallization of the stoichiometric forms of the p-toluenesulfonamide / triphenylphosphine oxide (p-TSATPPO) co-crystal system with acetonitrile have studied [9, 10]. A through literature search reveals there is no chemical computation on title compound has been carried out so far. In the present paper, we investigate vibrational spectra to identify the normal modes of vibration with potential energy distribution (PED) calculation. UV-Visible and NMR spectroscopy are performed to calculate the absorbtion maxima and chemical shift values. Electron density regions are identified through ESP surface. Hyperconjucative interaction are found by NBO analysis. To study the biological interaction of title ligand, docking procedure is carried out with SARS-CoV-2 virus protein.

2. Computational Methods

Molecular geometric optimization, and vibrational frequencies for NEPTS in gas phase are carried out at the 6-31G++(d,p) B3LYP level of theory with the help of Gaussian-09W package program [11]. PED's is calculated by using veda4 program [12]. HOMO-LUMO structures and ESP surface for NEPTS are obtained at same level theory and visualized using Gaussview5 program [13]. The HOMO-LUMO orbital energies are used to calculate chemical hardness, Electronic chemical potential and electrophilicity using the following equations (Eqs 1- 4) of CDFT. The hardness, chemical potential, and electro negativity values are calculated using Pearsons methods.

$$\eta = -(\varepsilon\text{HOMO} - \varepsilon\text{LUMO})/2 \tag{2.1}$$

$$\mu = (\varepsilon\text{HOMO} + \varepsilon\text{LUMO})/2 \tag{2.2}$$

$$\chi = \mu = (\varepsilon\text{HOMO} + \varepsilon\text{LUMO})/2. \tag{2.3}$$

The electrophilicity index is calculated using the method suggested by Parr et al [14].

$$\omega = \chi^2/2\eta. \tag{2.4}$$

Autodock tool was used to perform the MD studies and Pymol is used to visualized the p-l interaction [15, 16].

3. Result and Discussion

3.1. Molecular Geometry

The molecular structure of N-ethyl-P-toluenesulfonamide belongs to and in Fig.1 optimized geometric molecular structure of NEPTS is visualized and the structural parameters are enlisted in table 1. The bond length 1.4461, 1.448, 1.7266, 1.7722,

1.4535, and 1.0201 Å of S1-O2, S1-O3, S1-N4, S1-C5, N4-C6, and N4-H14, respectively and the corresponding bond lengths computed by HF method are 1.4232, 1.4239, 1.6303, 1.7725, 1.4615, 0.9985 Å. The highest bond length (1.7722 Å) was found between S1-C5. The bond angle 124.9754, 105.7842, 109.9948, 104.8534, 109.4083, 98.2434, 125.4034, 113.7605, and 118.7698° of O2-S1-O3, O2-S1-N4, O2-S1-C5, O3-S1-N4, O3-S1-C5, N4-S1-C5, S1-N4-C6, S1-N4-H14, and C6-N4-H14. The optimized molecular structure is shown in Fig. 1. The comparison values of DFT and HF methods are shown in Table 1.

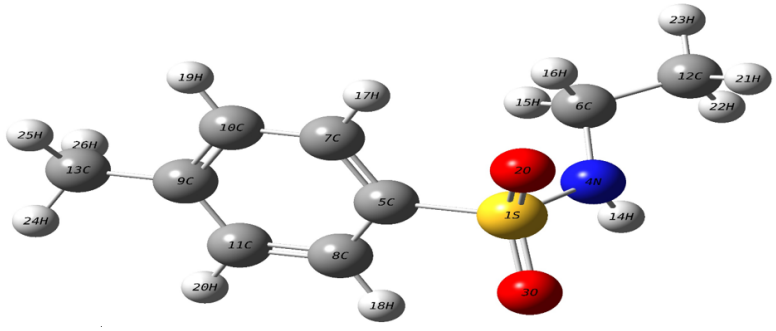

Figure 1: The Optimized Geometrical Structure with Labeling of Title Compound

Table 1: Optimized Bond Length and Bond Angle of Title Compound by DFT and HF Methods

Bond length(Å)	DFT	HF	Bond length(Å)	DFT	HF	Bond length(Å)	DFT	HF
S1-O2	1.446	1.423	O2-S1-O3	124.975	121.660	C11-C9-C13	120.557	120.262
S1-O3	1.448	1.424	O2-S1-N4	105.784	107.016	C7-C10-C9	121.070	121.031
S1-N4	1.727	1.630	O2-S1-C5	109.995	107.036	C7-C10-H19	119.701	119.154
S1-C5	1.772	1.773	O3-S1-N4	104.853	105.370	C9-C10-H19	119.226	119.813
N4-C6	1.454	1.462	O3-S1-C5	109.408	107.531	C8-C11-C9	121.000	121.029
N4-H14	1.020	0.999	N4-S1-C5	98.243	107.543	C8-C11-H20	119.709	119.307
C5-C7	1.411	1.382	S1-N4-C6	125.403	121.525	C9-C11-H20	119.287	119.660
C5-C8	1.413	1.389	S1-N4-H14	113.761	111.426	C6-C12-H21	110.594	110.704
C6-C12	1.546	1.521	C6-N4-H14	118.770	115.782	C6-C12-H22	111.490	111.287
C6-H15	1.095	1.088	S1-C5-C7	119.271	120.019	C6-C12-H23	107.792	109.882
C6-H16	1.090	1.081	S1-C5-C8	119.068	119.613	H21-C12-H22	109.447	108.395
C7-C10	1.377	1.387	C7-C5-C8	121.642	120.367	H21-C12-H23	109.033	108.739

C7-H17	1.083	1.074	N4-C6-C12	111.309	109.816	H22-C12-H23	108.415	107.744
C8-C11	1.377	1.379	N4-C6-H15	107.451	111.225	C9-C13-H24	111.942	110.570
C8-H18	1.083	1.074	N4-C6-H16	107.952	107.410	C9-C13-H25	109.156	111.290
C9-C10	1.419	1.387	C12-C6-H15	109.960	110.138	C9-C13-H26	111.966	110.941
C9-C11	1.417	1.394	C12-C6-H16	110.572	110.125	H24-C13-H25	106.932	108.010
C9-C13	1.491	1.509	H15-C6-H16	109.517	108.072	H24-C13-H26	109.677	107.675
C10-H19	1.084	1.076	C5-C7-C10	118.652	119.519	H25-C13-H26	106.916	108.221
C11-H20	1.084	1.076	C5-C7-H17	120.096	119.934			
C12-H21	1.090	1.084	C10-C7-H17	121.230	120.539			
C12-H22	1.092	1.087	C5-C8-C11	118.718	119.536			
C12-H23	1.092	1.085	C5-C8-H18	120.079	120.025			
C13-H24	1.091	1.086	C11-C8-H18	121.179	120.425			
C13-H25	1.100	1.083	C10-C9-C11	118.918	118.513			
C13-H26	1.091	1.085	C10-C9-C13	120.506	121.216			

3.2. Vibrational Assignments

The title compound NEPTS comprises of 26 atoms, giving rise to 72 vibrational modes. PED assignments have been carried out for theoretically predicted wavenumbers with DFT method. Scaling factor 0.961 was used for predicted wavenumbers [11] which can be useful to correlate the experimental results. The theoretical FT-IR and FT-Raman spectra for the NEPTS compound are shown in Figs. 2 and 3. Table 2 shows the Vibrational modes, unscaled, scaled frequencies with complete vibrational assignments based on the percentage PED.

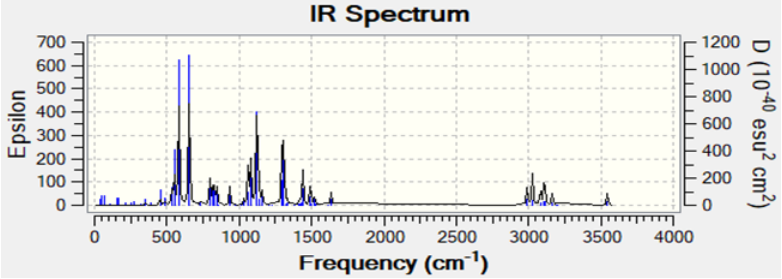

Figure 2: Theoretical IR Spectra of Title Compound

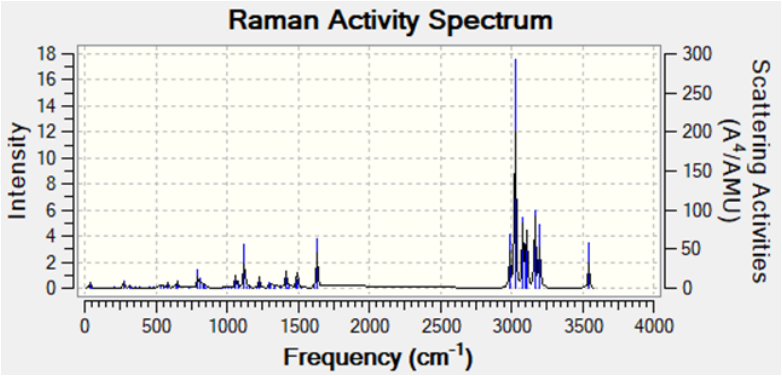

Figure 3: Theoretical Raman Spectra of the Title Compound

Table 2: Theoretical Scaled IR and Raman Intensities of Title Compound

MODES	UNSCLAED	SCALED	IR INTENSITIES	RAMAN INTENSITIES	PED ASSIGNMENTS
72	3546	3407	5	19	γNH(100)
71	3203	3078	0	26	γCH(95)
70	3195	3070	0	27	γCH(93)
69	3167	3044	3	33	γCH(94)
68	3165	3041	3	32	γCH(92)
67	3113	2992	5	18	γCH(98)
66	3108	2987	3	22	γCH(99)
65	3103	2982	4	18	γCH(99)
64	3083	2963	3	26	γCH(99)
63	3080	2960	4	30	γCH(100)
62	3029	2910	6	62	γCH(100)
61	3025	2907	5	97	γCH(100)
60	2991	2874	8	22	γCH(96)
59	1636	1572	4	21	γCC(39)
58	1612	1549	0	2	γCC(51)
57	1523	1464	1	1	γCC(21) +βCCC(13)
56	1522	1462	4	1	βHCH(50) +βHCC(50)
55	1500	1441	1	3	βHCH(70) +τHCCN(12)
54	1493	1435	6	2	βHCH(53)
53	1493	1434	1	4	βHCH(72)
52	1490	1432	2	3	βHCH(78) +τHCCC(12)

51	1440	1384	11	1	βHNC(45) +τHCNS(25)
50	1427	1371	1	0	γCC(28) +βHCC(25)
49	1417	1361	0	7	βHCH(93)
48	1415	1360	1	0	βHCH(87)
47	1380	1326	1	1	βHCC(44) +βHNC(17) +τHCNS(16)
46	1335	1283	1	0	γCC(43) +βHCC(10)
45	1328	1276	0	0	γCC(29) +βHCC(66)
44	1307	1256	28	1	γSO(33) +βHCC(17) +τHCNS(11)
43	1294	1244	14	2	γSO(32) +τHCNS(26) +βHNC(10) +βHCC(12)
42	1228	1180	0	5	γCC(48) +βCCC(14)
41	1205	1158	0	1	γCC(13) +βHCC(73)
40	1157	1112	4	0	τHCCN(42)
39	1136	1092	2	1	γCC(28) +βHCC(36)
38	1134	1090	3	0	γNC(19) +βCCN(12) +τHCCN(22)
37	1123	1079	47	18	γSC(10) +γSO(48)
36	1078	1036	17	2	γCC(33) +γSO(39)
35	1062	1020	5	2	γCC(12) +τHCCC(35) +βHCH(12)
34	1061	1019	6	4	γNC(25) +γCC(38) +τHCCC(12)
33	1033	993	2	0	βCCC(75)
32	1009	969	0	0	τHCCC(49) +γCC(10) +βHCH(11)
31	993	955	0	0	τHCCS(50) +τHCCC(36)
30	975	937	0	0	τHCCS(53) +τHCCC(19)
29	934	898	6	0	γSN(11) +τHCCN(23) +γNC(20) +γCC(33)

28	855	821	0	0	τHCCC(53) +τHCCS(44)
27	845	812	6	1	γSN(20) +τHCNS(14)
26	829	797	7	1	τHCCC(45) +τHCCS(31)
25	815	784	7	4	γCC(14) +βCCC(27)
24	796	765	10	8	γSN(21) +βCCC(11) +τHCNS(11)
23	729	700	1	0	τCCCC(69)
22	655	629	44	2	γSC(19) +OUTONOS(24) +γCC(13) +βCCC(11)
21	648	622	0	2	βCCC(60) +γCC(10)
20	582	559	38	3	βOSO(10) +τHNCC(24)
19	552	530	14	1	βNSC(15)τHNCC(14)
18	534	513	4	1	OUTONOS(34) +τHNCC(13) +βCCC(11)
17	483	465	2	0	βOSN(13) +OUTCCCC(24) +OUTSCCC(10)
16	454	436	3	1	βSCC(11) +OUTONCS(22) +βOSO(28)
15	416	400	0	0	τCCCC(89)
14	386	371	0	0	βCCC(25) +βOSN(33)
13	352	339	1	1	βNSC(12) +βOSO(23)
12	326	313	0	0	βCCC(10) +βCCN(19) +OUTCCCC(13) +βNSC(10)
11	318	306	0	1	OUTONCS(23) +βCCC(30)
10	274	263	0	3	γSC(48) +OUTONOS(14)

9	253	243	0	0	τHCCN(77)
8	210	202	0	0	βCNS(12) +OUTCCCC(11) +βNSC(17)
7	163	157	1	0	βSCC(46) +OUTONCS(12)
6	153	147	1	0	τCNSC(10) +βCNS(34) +βSCC(12) +OUTONCS(14)
5	103	99	0	0	τCNSC(36) +OUTSCCC(12) +τCCCC(15)
4	70	68	0	0	τCCNS(38) +τCNSC(24)
3	46	44	0	1	τNSCC(25) +τCCNS(19) +OUTSCCC(18) +βNSC(15)
2	39	37	0	0	τHCCC(64) +τNSCC(10) +τHCCC(21)
1	37	35	0	2	τCCNS(14) +τNSCC(57) +τCNSC(10)

3.2.1 NH Vibration

Usually, the N-H stretching vibrations are around 3500-3300 cm^{-1} [17]. In the present molecule, NH-stretching vibration (scaled) is only found at 3407 cm^{-1} in FT-IR with PED 100%. The NH stretching vibrational frequency is maximum in all other molecular vibrations and the NH bond length very less compared to others.

3.2.2 CH Vibrations

The regions for the identification of CH-stretching vibrations appear in the range of 3100-3000 cm^{-1} in the aromatic compounds. In present work, the calculated wave numbers are at 3078, 3070, 3044, and 3041 cm^{-1} with PED contribution of 95, 93, 94, and 92% respectively.

3.2.3 S=O Vibration

The molecule containing carbonyl group shows a strong absorption band. In present study, at mode no. 36 and 37 a strong S=O stretching vibrations (mixed) is observed. The calculated wave numbers are 1079 and 1036 cm^{-1}.

3.3. UV-Vis Spectra

The UV-Vis spectrum of the NEPTS compound as shown Fig. 4, is measured in gas phase. The calculated absorption wavelengths, electronic values, and oscillator strength are tabulated in Table 3. The absorption max are observed 246nm. The HOMO-LUMO contribution of the first transition was 97%, which reflect the considerably maximum oscillator value and high stabilization energy for this transition. The energy gap between the HOMO and the LUMO of the NEPTS compound was found to be 5.8783eV. And it is a critical parameter in determining molecular electrical transport properties because it is a measure of electron conductivity [18].

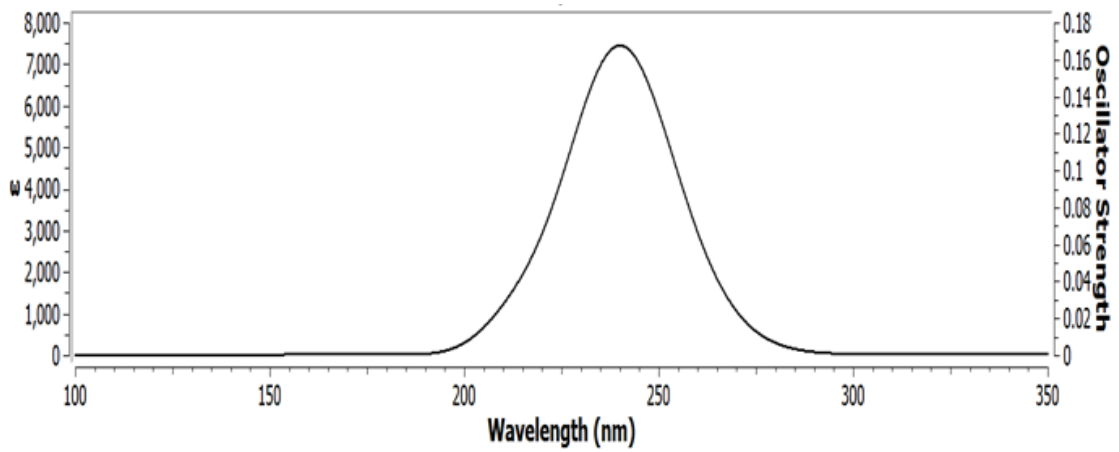

Figure 4: Theoretical UV-Vis Spectra of Title Compound

3.4. NMR

NMR spectral study is one of the main approaches in the conformation analysis related to the structure of the compound. In the present study, ^{1}H and ^{13}C NMR were carried out. For the theoretical scrutiny, GIAO-Gauge invariant atomic orbital is used along with DFT method. It is commonly used for the calculation of nuclear magnetic shielding tensor [19]. Both the theoretical study has been carried out in gas phase. The results are shown in Table 4. Chemical shifts 165 and 160ppm for C12, C13 is found to be higher. The proton NMR vaules are shown in Fig. 6The majority of carbon atoms are within 100ppm.

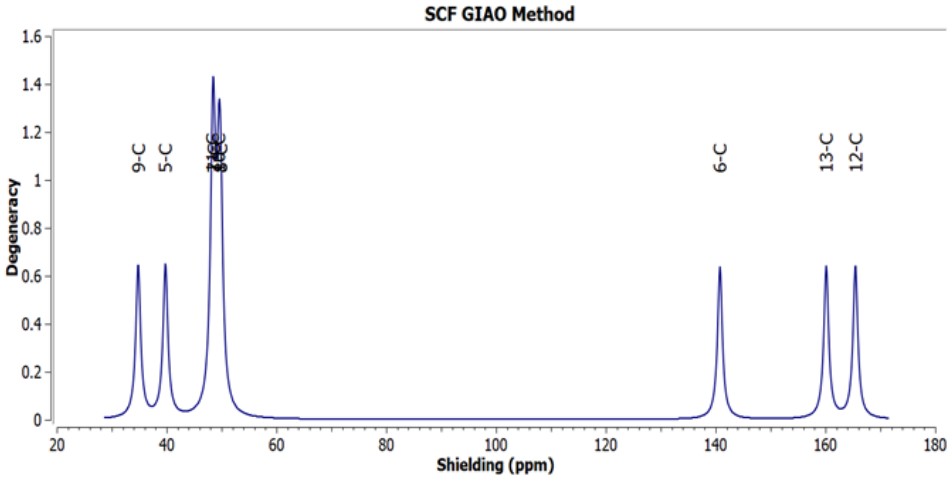

Figure 5: Theoretical ^{13}C NMR Spectra of Title Compound

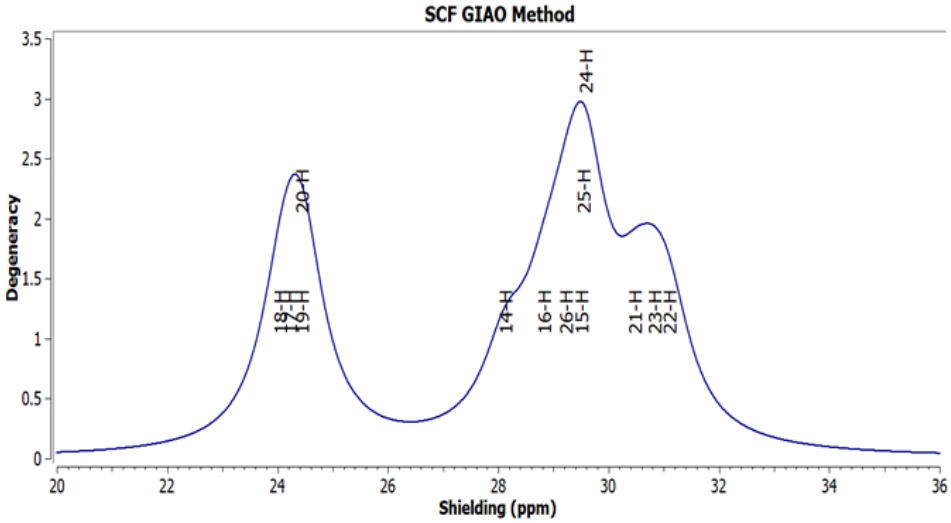

Figure 6: Theoretical 1H NMR Spectra of Title Compound

3.5. MEP Surface

Molecular electrostatic potential surface gives a clear image of the distribution of charge at surface (in and around) of the title compound in three dimensions. By doing so, the chemical bonds and nature of interactions can be identified. Colour ranging helps us to classify positive and negative regions effortlessly [31]. Fig. 7 shows the MESP map for the title compound. O atom has the highest electrophilicity, while hydrogen atoms have the highest nucleophilicity as indicated by red and blue colour. Usually, neutral regions are shown in green

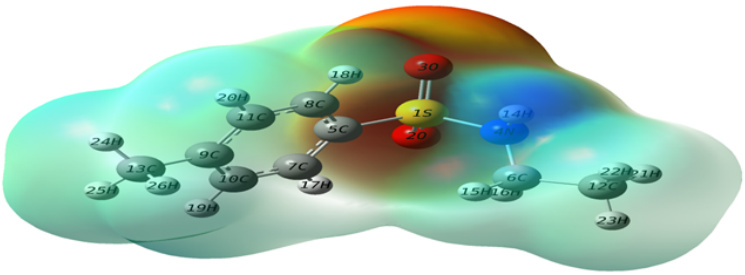

Figure 7: MEPS of Title Compound

3.6. NBO

The NBO studies are the most effective method for finding the intramolecular bonding, stability, transfer of charge and conjugative interactions in the molecular system [20]. The second order fock matrix was completed to compute the donor-acceptor exchanges in the NBO study [21]. In present molecule, strongest stabilization value is calculated for the donor bond πC9-C10 with the occupancy of 1.6337 and its anti-bonding π^*C5-C7 with the occupancy of 0.3838. The highest energy (E(2)) is 25.17 kJ/mol. A stabilization energy of 19.14 kcal/mol was observed in O2 (LP(3)) and S1-O3 with σ^* interaction.

Table 3: Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis of Title Compound

Type	Donor NBO (i)	Type	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
BD (1)	S 1 - O 2	BD*(1)	S 1 - O 2	0.65	1.27	0.027
BD (1)	S 1 - O 2	BD*(1)	S 1 - O 3	0.82	1.27	0.03
BD (1)	S 1 - O 2	BD*(1)	S 1 - N 4	1.62	1.12	0.04
BD (1)	S 1 - O 2	BD*(1)	S 1 - C 5	0.82	1.14	0.029
BD (1)	S 1 - O 2	BD*(1)	N 4 - H 14	0.72	1.38	0.028
BD (1)	S 1 - O 2	BD*(1)	C 5 - C 8	0.93	1.54	0.034
BD (1)	S 1 - O 3	BD*(1)	S 1 - O 2	0.83	1.27	0.03
BD (1)	S 1 - O 3	BD*(1)	S 1 - O 3	0.62	1.27	0.026
BD (1)	S 1 - O 3	BD*(1)	S 1 - N 4	1.72	1.12	0.042
BD (1)	S 1 - O 3	BD*(1)	S 1 - C 5	0.76	1.14	0.028
BD (1)	S 1 - O 3	BD*(1)	N 4 - C 6	0.99	1.31	0.032
BD (1)	S 1 - O 3	BD*(1)	C 5 - C 7	0.85	1.54	0.032
BD (1)	S 1 - N 4	BD*(1)	S 1 - O 2	2.5	1.06	0.047
BD (1)	S 1 - N 4	BD*(1)	S 1 - O 3	2.64	1.06	0.049
BD (1)	S 1 - N 4	BD*(1)	S 1 - N 4	1.15	0.91	0.031
BD (1)	S 1 - N 4	BD*(1)	S 1 - C 5	0.82	0.92	0.026

BD (1)	S 1 - N 4	BD*(2)	C 5 - C 7	0.97	0.78	0.027
BD (1)	S 1 - N 4	BD*(1)	C 6 - C 12	1.29	1.15	0.034
BD (1)	S 1 - C 5	BD*(1)	S 1 - O 2	2.47	0.97	0.045
BD (1)	S 1 - C 5	BD*(1)	S 1 - O 3	2.36	0.97	0.044
BD (1)	S 1 - C 5	BD*(1)	S 1 - N 4	2.45	0.82	0.042
BD (1)	S 1 - C 5	BD*(1)	S 1 - C 5	0.94	0.84	0.026
BD (1)	S 1 - C 5	BD*(1)	C 7 - C 10	2.62	1.25	0.051
BD (1)	S 1 - C 5	BD*(1)	C 8 - C 11	2.6	1.26	0.051
BD (1)	N 4 - C 6	BD*(1)	S 1 - O 3	0.67	1.05	0.024
BD (1)	N 4 - C 6	BD*(1)	C 12 - H 23	0.98	1.16	0.03
BD (1)	N 4 - H 14	BD*(1)	S 1 - O 2	1.63	0.95	0.036
BD (1)	N 4 - H 14	BD*(1)	C 6 - H 16	1.33	1.07	0.034
BD (1)	C 5 - C 7	BD*(1)	C 5 - C 8	4.24	1.29	0.066
BD (1)	C 5 - C 7	BD*(1)	C 7 - C 10	2.87	1.3	0.055
BD (1)	C 5 - C 7	BD*(1)	C 7 - H 17	1.28	1.17	0.035
BD (1)	C 5 - C 7	BD*(1)	C 8 - H 18	2.32	1.17	0.047
BD (1)	C 5 - C 7	BD*(1)	C 10 - H 19	2.19	1.16	0.045
BD (2)	C 5 - C 7	BD*(1)	S 1 - O 3	1.03	0.56	0.022
BD (2)	C 5 - C 7	BD*(1)	S 1 - N 4	4.47	0.41	0.039
BD (2)	C 5 - C 7	BD*(2)	C 8 - C 11	21.4	0.3	0.071
BD (2)	C 5 - C 7	BD*(2)	C 9 - C 10	15.85	0.3	0.062
BD (1)	C 5 - C 8	BD*(1)	C 5 - C 7	4.23	1.29	0.066
BD (1)	C 5 - C 8	BD*(1)	C 7 - H 17	2.32	1.17	0.047
BD (1)	C 5 - C 8	BD*(1)	C 8 - C 11	2.9	1.3	0.055
BD (1)	C 5 - C 8	BD*(1)	C 8 - H 18	1.26	1.17	0.034
BD (1)	C 5 - C 8	BD*(1)	C 11 - H 20	2.2	1.16	0.045
BD (1)	C 6 - C 12	BD*(1)	S 1 - N 4	3.26	0.76	0.047
BD (1)	C 6 - C 12	BD*(1)	C 6 - H 16	0.58	1.03	0.022
BD (1)	C 6 - H 15	BD*(1)	C 12 - H 21	2.48	0.92	0.043
BD (1)	C 6 - H 16	BD*(1)	N 4 - H 14	3.73	0.9	0.052
BD (1)	C 6 - H 16	BD*(1)	C 12 - H 22	2.66	0.9	0.044
BD (1)	C 7 - C 10	BD*(1)	S 1 - C 5	3.84	0.86	0.054
BD (1)	C 7 - C 10	BD*(1)	C 5 - C 7	3.65	1.27	0.061
BD (1)	C 7 - C 10	BD*(1)	C 7 - H 17	1.09	1.15	0.032
BD (1)	C 7 - C 10	BD*(1)	C 9 - C 10	3.27	1.28	0.058
BD (1)	C 7 - C 10	BD*(1)	C 9 - C 13	3.52	1.12	0.056
BD (1)	C 7 - C 10	BD*(1)	C 10 - H 19	0.93	1.14	0.029
BD (1)	C 7 - H 17	BD*(1)	C 5 - C 7	0.89	1.09	0.028
BD (1)	C 7 - H 17	BD*(1)	C 5 - C 8	4.66	1.09	0.064

BD (1)	C 7 - H 17	BD*(1)	C 7 - C 10	0.77	1.1	0.026
BD (1)	C 7 - H 17	BD*(1)	C 9 - C 10	3.55	1.1	0.056
BD (1)	C 7 - H 17	BD*(1)	C 10 - H 19	0.54	0.96	0.02
BD (1)	C 8 - C 11	BD*(1)	S 1 - C 5	3.75	0.86	0.053
BD (1)	C 8 - C 11	BD*(1)	C 5 - C 8	3.67	1.27	0.061
BD (1)	C 8 - C 11	BD*(1)	C 8 - H 18	1.11	1.15	0.032
BD (1)	C 8 - C 11	BD*(1)	C 9 - C 11	3.26	1.28	0.058
BD (1)	C 8 - C 11	BD*(1)	C 9 - C 13	3.46	1.12	0.056
BD (1)	C 8 - C 11	BD*(1)	C 11 - H 20	0.95	1.14	0.029
BD (2)	C 8 - C 11	BD*(2)	C 5 - C 7	18.74	0.27	0.065
BD (2)	C 8 - C 11	BD*(2)	C 9 - C 10	21.89	0.29	0.071
BD (1)	C 8 - H 18	BD*(1)	C 5 - C 7	4.58	1.09	0.063
BD (1)	C 8 - H 18	BD*(1)	C 5 - C 8	0.84	1.09	0.027
BD (1)	C 8 - H 18	BD*(1)	C 8 - C 11	0.78	1.1	0.026
BD (1)	C 8 - H 18	BD*(1)	C 9 - C 11	3.58	1.09	0.056
BD (1)	C 8 - H 18	BD*(1)	C 11 - H 20	0.54	0.96	0.02
BD (1)	C 9 - C 10	BD*(1)	C 7 - C 10	3.08	1.28	0.056
BD (1)	C 9 - C 10	BD*(1)	C 7 - H 17	2.09	1.15	0.044
BD (1)	C 9 - C 10	BD*(1)	C 9 - C 11	3.09	1.27	0.056
BD (1)	C 9 - C 10	BD*(1)	C 9 - C 13	1.6	1.12	0.038
BD (1)	C 9 - C 10	BD*(1)	C 10 - H 19	0.99	1.14	0.03
BD (1)	C 9 - C 10	BD*(1)	C 11 - H 20	2.51	1.14	0.048
BD (1)	C 9 - C 10	BD*(1)	C 13 - H 24	0.54	1.1	0.022
BD (2)	C 9 - C 10	BD*(2)	C 5 - C 7	25.17	0.27	0.074
BD (2)	C 9 - C 10	BD*(2)	C 8 - C 11	18.21	0.28	0.065
BD (2)	C 9 - C 10	BD*(1)	C 13 - H 24	1.37	0.65	0.03
BD (2)	C 9 - C 10	BD*(1)	C 13 - H 26	3.05	0.65	0.044
BD (1)	C 9 - C 11	BD*(1)	C 8 - C 11	3.07	1.28	0.056
BD (1)	C 9 - C 11	BD*(1)	C 8 - H 18	2.12	1.14	0.044
BD (1)	C 9 - C 11	BD*(1)	C 9 - C 10	3.07	1.27	0.056
BD (1)	C 9 - C 11	BD*(1)	C 9 - C 13	1.55	1.11	0.037
BD (1)	C 9 - C 11	BD*(1)	C 10 - H 19	2.55	1.14	0.048
BD (1)	C 9 - C 11	BD*(1)	C 11 - H 20	0.96	1.13	0.03
BD (1)	C 9 - C 11	BD*(1)	C 13 - H 25	0.64	1.1	0.024
BD (1)	C 9 - C 13	BD*(1)	C 7 - C 10	2.52	1.21	0.049
BD (1)	C 9 - C 13	BD*(1)	C 8 - C 11	2.5	1.21	0.049
BD (1)	C 9 - C 13	BD*(1)	C 9 - C 10	1.81	1.21	0.042
BD (1)	C 9 - C 13	BD*(1)	C 9 - C 11	1.77	1.2	0.041
BD (1)	C 9 - C 13	BD*(1)	C 13 - H 26	0.54	1.03	0.021

BD (1)	C 10 - H 19	BD*(1)	C 5 - C 7	3.79	1.09	0.057
BD (1)	C 10 - H 19	BD*(1)	C 7 - C 10	0.62	1.1	0.023
BD (1)	C 10 - H 19	BD*(1)	C 9 - C 10	0.86	1.09	0.027
BD (1)	C 10 - H 19	BD*(1)	C 9 - C 11	4.41	1.09	0.062
BD (1)	C 11 - H 20	BD*(1)	C 5 - C 8	3.82	1.08	0.058
BD (1)	C 11 - H 20	BD*(1)	C 8 - C 11	0.64	1.1	0.024
BD (1)	C 11 - H 20	BD*(1)	C 8 - H 18	0.51	0.96	0.02
BD (1)	C 11 - H 20	BD*(1)	C 9 - C 10	4.37	1.09	0.062
BD (1)	C 11 - H 20	BD*(1)	C 9 - C 11	0.82	1.09	0.027
BD (1)	C 12 - H 21	BD*(1)	C 6 - H 15	2.47	0.89	0.042
BD (1)	C 12 - H 22	BD*(1)	C 6 - H 16	2.33	0.91	0.041
BD (1)	C 12 - H 23	BD*(1)	N 4 - C 6	3.7	0.83	0.05
BD (1)	C 13 - H 24	BD*(1)	C 9 - C 10	3.45	1.08	0.055
BD (1)	C 13 - H 24	BD*(2)	C 9 - C 10	1.57	0.54	0.028
BD (1)	C 13 - H 25	BD*(2)	C 9 - C 10	0.54	0.54	0.017
BD (1)	C 13 - H 25	BD*(1)	C 9 - C 11	4.07	1.08	0.059
BD (1)	C 13 - H 26	BD*(1)	C 9 - C 10	0.82	1.08	0.027
BD (1)	C 13 - H 26	BD*(2)	C 9 - C 10	4.63	0.53	0.048
LP (1)	O 2	BD*(1)	S 1 - O 3	1.84	1.1	0.041
LP (1)	O 2	BD*(1)	S 1 - C 5	0.62	0.97	0.023
LP (2)	O 2	BD*(1)	S 1 - O 3	2.23	0.58	0.032
LP (2)	O 2	BD*(1)	S 1 - N 4	10.47	0.43	0.061
LP (2)	O 2	BD*(1)	S 1 - C 5	16.26	0.44	0.076
LP (2)	O 2	BD*(1)	C 5 - C 8	0.66	0.85	0.022
LP (3)	O 2	BD*(1)	S 1 - O 3	19.14	0.58	0.096
LP (3)	O 2	BD*(1)	S 1 - N 4	13.14	0.43	0.067
LP (3)	O 2	BD*(1)	S 1 - C 5	1.17	0.44	0.02
LP (1)	O 3	BD*(1)	S 1 - O 2	1.85	1.1	0.042
LP (1)	O 3	BD*(1)	S 1 - C 5	0.67	0.97	0.024
LP (2)	O 3	BD*(1)	S 1 - O 2	2.1	0.58	0.031
LP (2)	O 3	BD*(1)	S 1 - N 4	10.3	0.43	0.06
LP (2)	O 3	BD*(1)	S 1 - C 5	16.23	0.44	0.076
LP (2)	O 3	BD*(1)	C 5 - C 7	0.57	0.85	0.02
LP (3)	O 3	BD*(1)	S 1 - O 2	19.52	0.58	0.096
LP (3)	O 3	BD*(1)	S 1 - N 4	12.32	0.43	0.065
LP (3)	O 3	BD*(1)	S 1 - C 5	1.25	0.44	0.021
LP (3)	O 3	BD*(1)	N 4 - C 6	0.5	0.61	0.016
LP (1)	N 4	BD*(1)	S 1 - O 2	2.38	0.61	0.034
LP (1)	N 4	BD*(1)	S 1 - O 3	1.34	0.61	0.026

LP (1)	N 4	BD*(1)	S 1 - C 5	7.35	0.48	0.054
LP (1)	N 4	BD*(2)	C 5 - C 7	0.95	0.33	0.017
LP (1)	N 4	BD*(1)	C 6 - C 12	0.9	0.7	0.023
LP (1)	N 4	BD*(1)	C 6 - H 15	6.61	0.71	0.062
LP (1)	N 4	BD*(1)	C 6 - H 16	1.48	0.73	0.03
BD*(1)	S 1 - O 2	BD*(1)	N 4 - C 6	0.52	0.04	0.013
BD*(1)	S 1 - O 2	BD*(1)	N 4 - H 14	1.24	0.1	0.036
BD*(1)	S 1 - O 2	BD*(1)	C 5 - C 8	0.72	0.27	0.043
BD*(1)	S 1 - O 3	BD*(1)	N 4 - C 6	3.85	0.04	0.037
BD*(1)	S 1 - O 3	BD*(1)	N 4 - H 14	0.7	0.1	0.027
BD*(1)	S 1 - O 3	BD*(1)	C 5 - C 7	0.65	0.27	0.042
BD*(1)	S 1 - N 4	BD*(1)	S 1 - C 5	7.91	0.02	0.021
BD*(1)	S 1 - N 4	BD*(1)	N 4 - C 6	1.77	0.19	0.045
BD*(1)	S 1 - N 4	BD*(1)	C 6 - C 12	0.56	0.24	0.03
BD*(1)	S 1 - C 5	BD*(1)	C 7 - C 10	1.03	0.42	0.056
BD*(1)	S 1 - C 5	BD*(1)	C 7 - H 17	1.42	0.29	0.054
BD*(1)	S 1 - C 5	BD*(1)	C 8 - C 11	1	0.42	0.055
BD*(1)	S 1 - C 5	BD*(1)	C 8 - H 18	1.46	0.29	0.055
BD*(2)	C 5 - C 7	BD*(1)	S 1 - O 3	0.51	0.28	0.021
BD*(2)	C 5 - C 7	BD*(1)	S 1 - N 4	5.05	0.13	0.041
BD*(2)	C 5 - C 7	BD*(2)	C 8 - C 11	246.97	0.01	0.08
BD*(2)	C 5 - C 7	BD*(2)	C 9 - C 10	192.78	0.02	0.084
BD*(2)	C 9 - C 10	BD*(1)	C 13 - H 26	1.48	0.37	0.05

3.7. Mulliken Charges

The calculation of atomic charges is an important feature in the field of quantum mechanical calculations to molecular systems. The charge distributions are calculated from Mulliken population analysis. The highest and lowest charges are calculated. The corresponding Mulliken plot values are shown in Fig. 8. C5 possesses the highest negative charges.

3.8. Docking

The molecular docking method was adopted to investigate protein ligand interaction. To find the antiviral activity of the NEPTS molecule SARS-CoV-2 6Y84 crystal structure is chosen to study the P-L interaction and it was downloaded from RCSB protein database (https://www.rcsb.org/). Molecular docking is a powerful computational tool in predicting the binding affinity of a ligand with protein. The calculated minimum binding energy of PL complex is 6.67 kcal/mol. The protein ligand interaction with distance and bonded residues are shown in Fig. 9

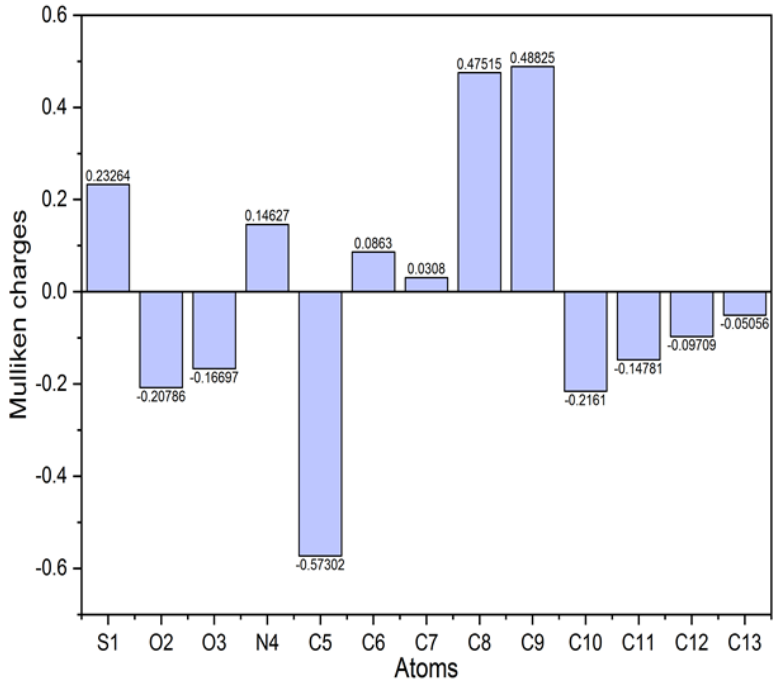

Figure 8: Mulliken Charges of Title Compound

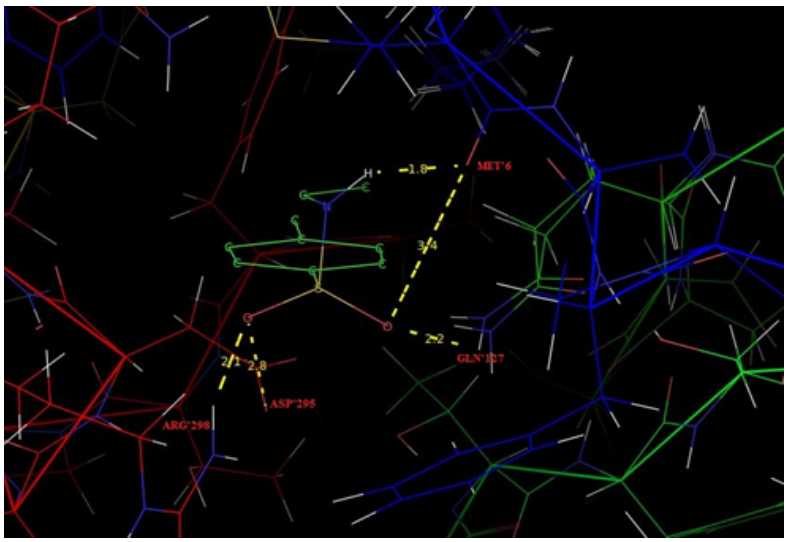

Figure 9: H-Bond Interaction of Title Compound with Receptor Protein

4. Conclusion

A complete molecular structure analysis has been reported based on the quantum mechanical approach by ab initio HF and DFT (B3LYP) calculations. Theoretical

spectroscopic (IR, Raman, UV-Vis and NMR) investigation have been discussed. NBO reflects the stabilization and charge transfer within the molecule. HOMO and LUMO orbital's energy have been computed. ^{13}C and ^{1}H NMR chemical shifts calculation of the N-ethyl-P-toluenesulfonamide molecule were carried out by using B3LYP functional with 6-311G++(d,p) basis set. Moreover, MEPS reveals the electrophilic and neucleophilic regions of the title molecule. Mulliken charges are also calculated. Molecular docking study reveals the NEPTS molecule is biologically active.

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SYNTHESIS AND CHARACTERIZATION OF IRON OXIDE NANOPARTICLES ON XANTHAN AND CARRAGEENAN TEMPLATES

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Abstract

Polysaccharides like xanthan and carrageenan have been employed as templates for the synthesis of iron oxide nanoparticles using co-precipitation method. The polysaccharides offer selective binding sites for Ferrous under aqueous condition. Precise temperature and subsequent removal of the templates enables the synthesis of nanoparticles. X ray diffraction (XRD) revealed the crystalline character and size of the magnetite nanoparticles were about 100nm. FT-IR results confirm the formation of Fe_3O_4 nanoparticles in biopolymer matrix. Analysis of the absorption coefficient has been carried out and the nature of transitions and the optical band gap Eg are determined.

Keywords: Polysaccharide, Co-precipitation, Xanthan, Carrageenan.

1. Introduction

In recent years, the rapid growth and evolution of technology have gained increasing attention and attracted tremendous interest from researchers worldwide in the fields [1] such as ultra high density data storages [2 – 4], sensors, drug delivery system [5 – 7], bullet proof vest and biochemical's due to its peculiar properties [8]. The key points of using polysaccharides are to achieve uniform dispersion of Fe_3O_4 in nano dimension and the choice of appropriate method for fabricating the nanomaterials.

Polysaccharides have found novel uses in green chemistry. Polysaccharides are a broad family of natural carbohydrates containing both glycosidically related sugar residues and amino acid-bound polymer saccharides. Its eco-friendly character [9 – 11], non-toxic [12 – 14], renewable and widely available in large quantities is the most significant feature. The variable polysaccharides [15] origin describes the richness of their structures and the related properties of xanthan, carrageenan, pectin, starch, etc.

Xanthan is a polysaccharide secreted by the bacterium Xanthomon as campestris, used as a food additive and rheology modifier, widely used as a food thickening agent (for example in salad dressings) and stabiliser (for example, to prevent separation of ingredients in cosmetic products). It is formed by fermentation of glucose, sucrose, or lactose [16].

Carrageenan, obtained by extraction from some species of red algae (Rhodophyta), is the common name for a family of polysaccharides. They are the ones who A mixture of water-soluble linear sulfated galactans consisting essentially of an alternating repeating unit of β-(1-3)-d-galactose (G-units) and alpha-(1-4)-d-galactose (D-units) or alpha-(1-4)-3,6-anhydro-d-galactose (DA units). The variation in this essential structure is the product of 3, 6-anhydrogalactose content, position and number of groups of sulphates. Sodium alginate is a natural linear polysaccharide, biocompatible, non-toxic, non-immunogenic and biodegradable, derived from a variety of brown seaweed species. Chemically, it is a block copolymer consisting of two separate repeating units, (1-4)-linked β-d-mannuronic acid (M) and alpha-l-guluronic acid (G) monomers, which, depending on the biological source, growth and stationary conditions, vary in quantity and sequential distribution along the polymer chain [17-20].

2. Experimental

2.1. Materials

All chemical reagents were analytical grade and used without further purification. $FeCl_3$ $6H_2O$, $FeCl_2$ $4H_2O$, $FeSo_4$ $7H_2O$, Xanthan, carrageenan , deionized water, aqueous ammonia and ethanol were purchased from M/s JAYSUN Chemical, India. The pH meter was employed to control the pH of the solution. The Laboratory Oven was used to dry the washed sample.

2.2. Synthesis of Fe_3O_4

Iron oxide (Fe_3O_4) were synthesized using co precipitate method by dissolving appropriate amount of ferrous chloride (Fe Cl_2 $4H_2O$) and ferric chloride (Fe Cl_3 $6H_2O$) in deionised water. The mixture was mixed slowly in aqueous ammonia solution with vigorous stirring for 30 minutes. The pH of the solution was maintained in between 11 and 12 using concentrated ammonium hydroxide solution. The resultant mixture was centrifuged to obtain the nanoparticles. The obtained precipitate was washed three times with distilled water and tetra hydrofurane (THF) and then dried in the air for a period of 12 hrs.

2.3. Synthesis of Xanthan

5g of xanthan was dissolved in 100 ml of de-ionized water in order to prepare iron oxide with the xanthan template. $FeSo_4.7H_2O$ was added to assess the volume of the

template solutions so that the polysaccharide and Fe ratio ranged from 1:4. The resulting solution was stirred for 30 minutes. The template-iron mixed solution was annealed at a temperature of 800°C with the heating rate of 5°C / min for 120 minutes. The temperature was allowed to fall at the rate of 10°C / min to room temperature.

2.4. Synthesis of Carrageenan

5g of Carrageenan was dissolved in 100 ml of water in order to prepare iron oxide with a Carrageenan template. $FeSo_4$ $7H_2O$ was added to know the volume of the template solutions such that the polysaccharide Fe ratio 1:4. The resulting solution was stirred for 30 minutes. The template-iron mixed solution was treated at 800°C and kept for 120 minutes at that temperature, after which it was cooled at a rate of 10°C/minutes to room temperature.

2.5. Characterization

The synthesized material was subjected to various characterizations. Powder X-ray diffraction (XRD) patterns were recorded by a Bruker Model: D8 Advance diffractometer with CuKα radiation (1.54Å) operating at 40 kV and 30mA.The IR spectra were obtained using a Perkin Elmer IR Spectrometer instrument at room temperature in the 4000400cm^{-1} range. The UV-Vis spectrum of Fe_3O_4 -NPs was determined using UV-Visible Spectrophotometer (UV-1800).

3. Results and Discussion

The Fe_3O_4 iron oxide was synthesised without and with xanthan and carrageenan polysaccharide templates.

3.1. FT IR Analysis

The iron oxide Fe_3O_4 templates xanthan and Carrageenan were subjected to FT-IR analysis without and with bio-polymers. The Fourier transform infrared of iron oxide absorption spectrum with and without bio-polymers is given as Fig (3.1.1) provides a range of reports on Xanthan FT-IR absorption studies showing characteristic peaks at 556-642, 1467-1095, 1707-1606, and 3525-3786 cm^{-1}. In Xanthan templates, the frequency number range of 556 present in C-I bond of vibration stretching mode is found. 642 cm^{-1} frequency number range present in (nitrogen-oxygen bond) C- Br shape of vibration stretching mode bond is found in iron oxide with Xanthan template. In Xanthan models, the frequency number range of 1707 cm^{-1} present in C = O compounds containing the vibration stretching mode bond is found. In Iron Oxide with Xanthan templates, the frequency number range of 1606 cm^{-1} present in C = O compounds containing the vibration stretching mode bond is found.

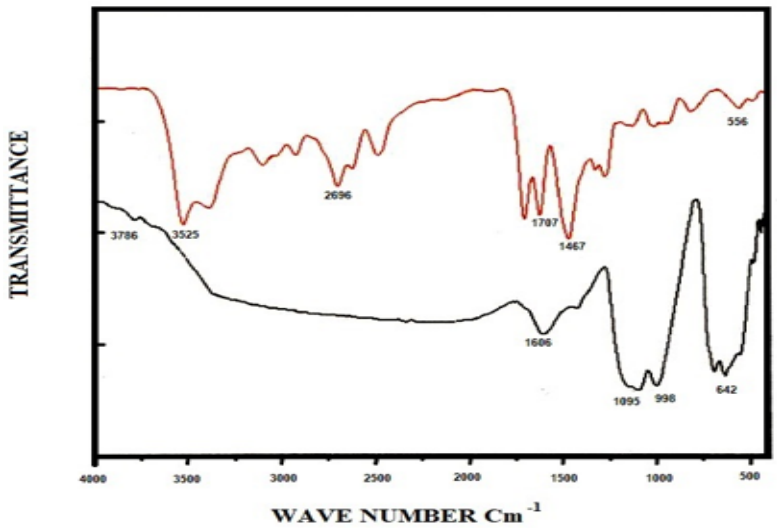

Figure 1: FT IR Spectrum of Xanthan and Iron Oxide with Xanthan Templates

The Fourier transform infrared of iron oxide absorption spectrum with and without bio-polymers is given as Figs. (3.1.2 & 3.1.3) provides the number of reports on the FT-IR absorption studies of Carrageenan showing characteristic peaks at 533-560, 1099-1383, 1422-1534, 1629-1700 and 3414-3423 cm^{-1}. The recorded characteristic peak of the Fe-O group of iron oxide located at 560 cm^{-1} in our sample. The peak of the Fe-O group of iron oxide located at 560.50 cm^{-1} iron oxide without templates in the synthesis of iron oxide with carrageenan templates the characteristic peak was reduced by 533.18 cm^{-1}. As iron oxide (Fe_3O_4), the-NH_2 stretching peaks at 3423.25 cm^{-1} are moved to 3429.05 cm^{-1} for iron oxide with carrageenan templates. When iron oxide (Fe_3O_4), the stretching of COOH peaks at 1629.23 cm^{-1} was moved to 1702.09 cm^{-1} for iron oxide with carrageenan templates.

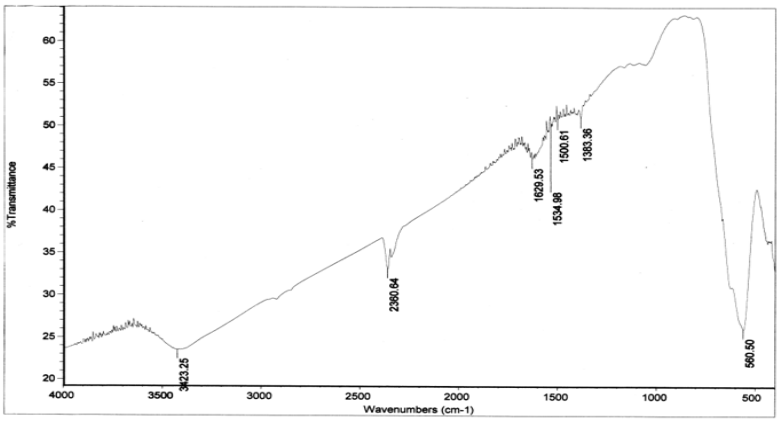

Figure 2: FT IR Spectrum Iron Oxide

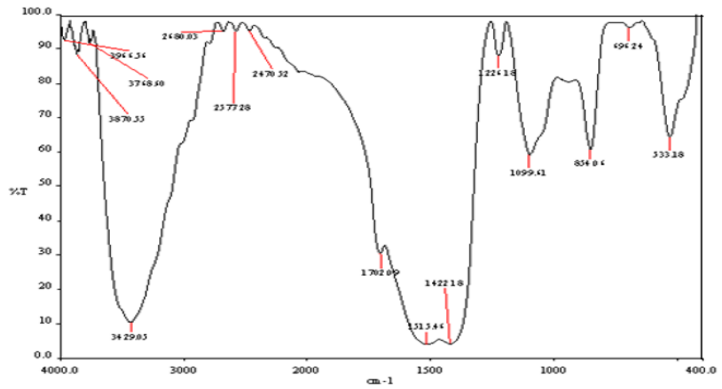

Figure 3: FT-IR Spectrum of Iron Oxide with Carrageenan Templates

4. XRD Analysis

An XRD analysis was performed on the iron oxide Fe_3O_4 with Xanthan and carrageenan biopolymer templates.

The XRD patterns of xanthan and carrageenan did not vary clearly between them, shown in Fig. 3.2.1 and 3.2.2. The powder XRD patterns also showed different peaks with values of approximately 30.11°, 35.31°, 43.15°, 57.25° and 63. 51° for carrageenan, for xanthan the 2θ values are approximately 30.16°, 35.47°, 43.22°, 57.11° and 62.86° respectively. These peak locations and relative peak intensities corresponded to the Fe_3O_4 peaks, so it was determined that xanthan and carrageenan magnetic Fe_3O_4 nano particles were successfully manufactured. Xanthan diffraction peaks showed wider FWHM than carrageenan (full width at half-maximum). The crystalline sizes could be determined from FWHM using the formula of scherrer expressed as D = 0.89 / ($\beta \cos \theta$) where β is the wavelength of the XRD peaks, β is FWHM and x is the angle of diffraction. The carrageenan Fe_3O_4 nano particles were clearly smaller than xanthan. Since no apparent polysaccharide crystallinity was observed, the polysaccharide portion was in the amorphous phase, which could be the Fe_3O_4 polysaccharide hydrophilicity.

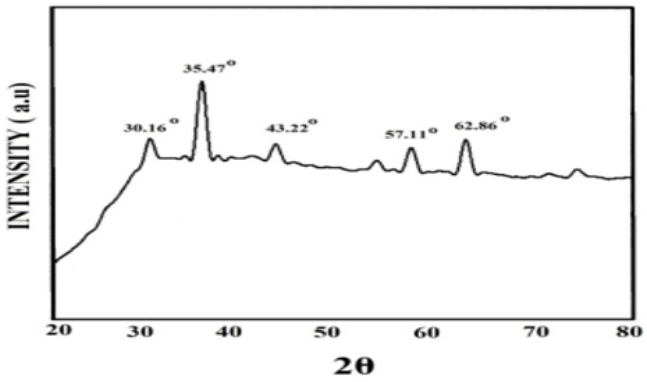

Figure 4: XRD Spectrum of Xanthan with Fe_3O_4

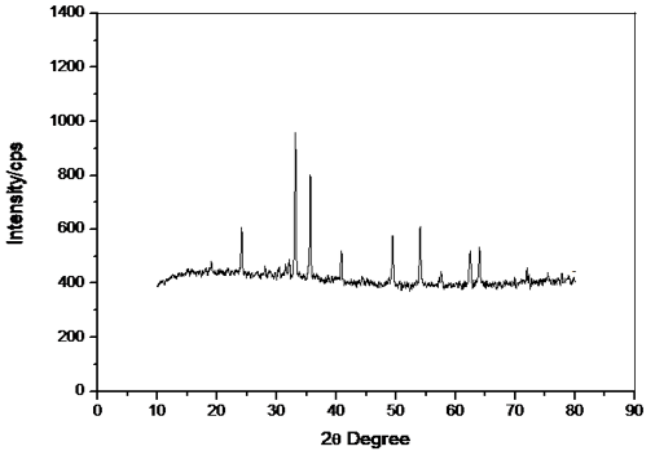

Figure 5: XRD Spectrum of Carrageenan with Fe_3O_4

4.1. UV Visible and Micro Structural Analysis

UV analysis was performed on the Biopolymer template xanthan with iron oxide without iron oxide. For biopolymer templates like xanthan and carrageenan with iron oxide without iron oxide, the spectral distributions of transmittance (T) dates are analysed in the spectral area (300-800 nm).

Analysis of the absorption coefficient has been carried out to determine the existence of the transitions involved and to obtain the distance in the optical band Eg involves plotting $(\alpha h\nu)^2$ against $h\nu$. Figure (3.3.3 & 3.3.4) shows that linear functions are the plots of $(\alpha h\nu)^2$ vs $h\nu$. This linearity indicates the presence of transitions permitted directly. The linear dependency extrapolation of both abscissa relationships gives the corresponding bandwidth Eg. The value of the optical energy gap with xanthan (2.52 eV), carrageenan (0.51 eV) models obtained for iron oxide.

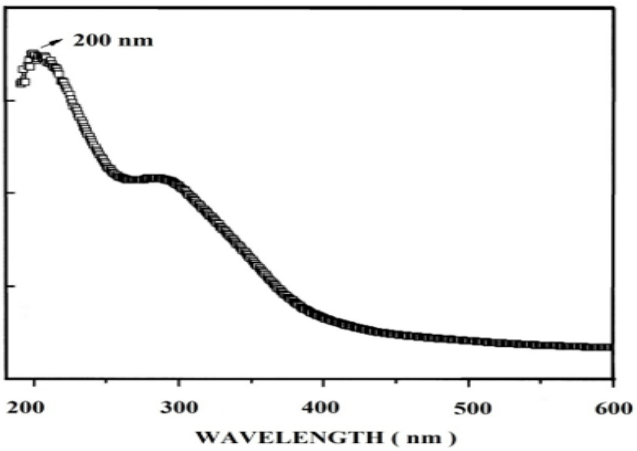

Figure 6: UV Spectrum of Xanthan with Fe_3O_4

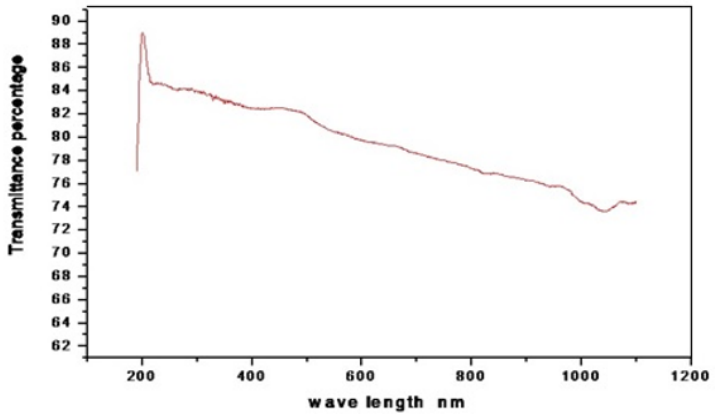

Figure 7: UV Spectrum of Carrageenan with Fe_3O_4

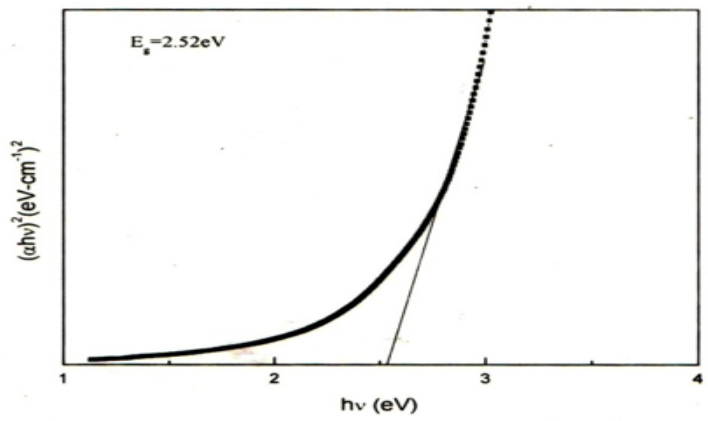

Figure 8: Plots of $(\alpha h\nu)^2$ versus hν Direct Transition of Xanthan / Fe_3O_4

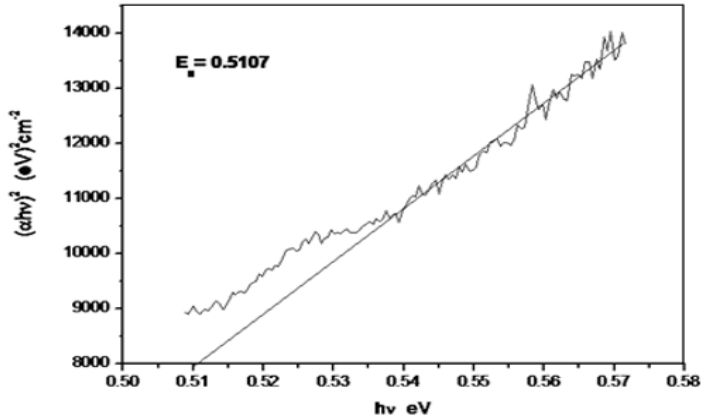

Figure 9: Plots of $(\alpha h\nu)^2$ versus hν Direct Transition of Carrageenan / Fe_3O_4

5. Summary and Conclusion

Polysaccharides like xanthan and carrageenan as templates for synthesis of iron oxide nanoparticles seems beneficial. The particles are highly crystalline and the XRD pattern matches with that of hematite. The particles of iron oxide obtained are of micro- to nano-dimensions with average size in the range of about 100 nm .The FT IR study confirm the formation of iron oxide. UV-Vis spectral analysis confirms the blue shift of the absorption edge and in turn, the reduction in particle size observed due to the treatment of polysaccharide templates.

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SYNTHESIS AND CHARACTERIZATION OF AROYLHYDRAZONE AND ANTICONVULSANT STUDY

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Abstract

The present study focused on synthesis of hydrazones for the development of newer pharmaceutical valuable compound. A highly effective medicinal hydrazide derivative (E)-N'-(2,4-dichlorobenzylidene) nicotinohydrazide have been synthesized from Schiffbase route. The prepared compound was characterized using Fourier Transform Infrared spectroscopy (FT-IR), and H^1 and C^{13} Nuclear Magnetic Resonance spectroscopy (NMR). The solubility of the compound was examined using different solvents. In addition, the purity of the prepared compound has been studied using Thin layer chromatography (TLC). The biological studies such as antioxidant activity was studied by Ferric rducinf ability of plasma (FRAP) method and anticonvulsant activity by Zebra fish by T-Maze model. The molecular docking study was conducted by in silico method by utilizing caspase-3 and 7.

Keywords: NMR, TLC, FRAP and NHN.

1. Introduction

The chemistry of coordination compounds can have a wide variety of structures and challenging the inorganic chemistry. Diverse coordination compounds synthesized from interesting ligand systems containing different donor groups. Aroylhydrazones, a class of azomethines widely employed as ligands in coordination chemistry. Amido form hydrazones are generally in solid state but in liquid phase, they exist as an equilibrium mixture of amido and iminol forms. The aroyl hydrazones contain combination of amide oxygen, an imine nitrogen moiety and extra donor site (usually N or O) generally from the aldehyde or ketone formed by Schiff base. The bioactivity of hydrazones is

depending on the type of multidentate coordination centers. Many aroylhydrazones derived from orthohydroxy aromatic aldehydes [1] and 2-N-heterocyclic aldehydes [2] have been studied extensively. Hydrazones with azomethine proton NH-N=CH is a class of important compounds evaluated for drug designing [3].

Hydrazones can be made by three main synthetic pathways (i) Japp-Klingemann reaction (ii) coupling of hydrazines and ketones or aldehydes (iii) coupling between aryl halides and non- substituted hydrazones. Condensation of aromatic hydrazides (aroylhydrazides) with carbonyl compounds is a simple chemical reaction responsible for formation of aroyl hydrazones [4, 5].

Hydrazones derived from ketones and aldehydes comes under the class of organic compounds with the structure, R_1R_2C =NNH_2. Aroyl hydrazones are a class of azomethines having the group -C=N-N- and are widely employed as ligands in coordination chemistry. These type of compounds are versatile, readily available with various functionalities depending on the nature of the starting materials employed for their preparation. The amido-iminol equilibrium largely depend on nature of the substituents, pH of the medium and the metal salts employed in synthesis pathway. The most potent property of aroylhydrazones is their great physiological activity due to the presence of the active pharmacophore (C=N-NH- CO) and provides a wide range of application in medicinal and pharmaceutical fields with various biological applications. Therefore, a number of hydrazone derivatives have been synthesized and experimentally tested against wide range of diseases.

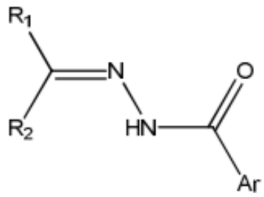

Figure 1: General Formula for a Substituted Aroylhydrazone

These compounds contain C = N bond, which is conjugated with a lone pair of electrons of the functional nitrogen atom, which is nucleophilic, and the carbon atom, has both electrophilic and nucleophilic nature. The combination of hydrazones with other functional group leads to compounds with unique physical properties plays important role in synthesis of heterocyclic compounds. The structure of a hydrazone generally made-up of nucleophilic imine and amino- nitrogen, an imine carbon, configurational isomerism stemming from the intrinsic nature of the C=N bond and an acidic N-H proton [6]. These azomethine -NHN=CH- is a proton constitute act as an important role in designing of new drug and development. Hydrazones are formed by the reaction of hydrazine or hydrazide with aldehydes and ketones [7].

2. Materials and Methods

2.1. Materials

All the chemicals used were of Merck and Sigma Aldrich products, available commercially in AR grade. The purchased chemicals were used without any further purification.

2.2. Preparation of (E)-N'-(2,4-Dichlorobenzylidene) Nicotinohydrazide

The synthetic method (Scheme 1) was adopted. The nicotinic acid hydrazide (10 mmol, 1.37g) was dissolved in 20 ml of absolute ethanol by heating gently on water bath. 0.875g of 2,4 dichloro benzaldehyde is taken in a clean conical flask. Then it is dissolved in 10ml of methanol. The above mixture was stirred at 20°C for 8 h and then it allowed to stand at ambient temperature for overnight. After 24h, the white precipitate is collected by filteration. The crude sample was recrystallized from ethanol. The purity of the compound was checked by Thin Layer Chromatography (TLC).

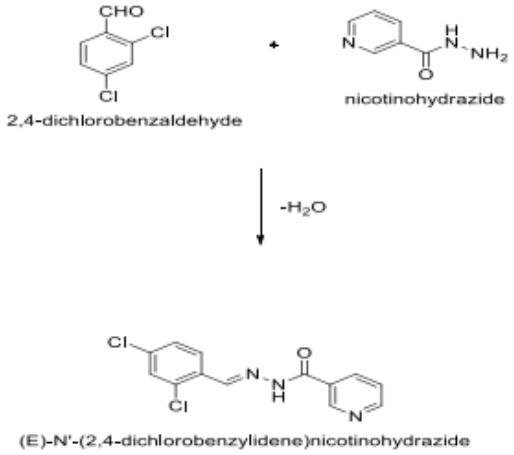

Figure 2: Scheme 1 - Structure of (E)-N-(2,4-Dichlorobenzylidene) Nicotinohydrazide.

2.3. Characterization Techniques

Some physical methods were used to elucidate the bonding and structure of the synthesized ligands and complexes and to confirm the expected properties. While the ligands were characterized by usual methods such as analytical technique such as TLC, spectral techniques such as IR, UV-Visible, NMR and mass spectral techniques, it differs for complexes depending on the nature of the ligands and the metal ions involved.

3. Results and Discussion

3.1. FT-IR Analysis

The IR spectrum of Schiff base showed characteristic broad band at 3248 cm^{-1} can be attributed to ν(N-H) and aromatic ν(ArC-H) stretching vibrations appeared at 3051 cm^{-1}. It is indicated that the Schiff base also having intermolecular O...H hydrogen bonding. Another distinctive vibration expected for N-N observed at 1918 cm^{-1}. Generally, carbonyl group stretching vibrations appears at 1680-1700 cm^{-1} but in this case appeared at 1629 cm^{-1}; this is due to amide group present in the compound, which decreases the carbonyl functional group. The newly generated C=N stretching vibration appeared at 1491 cm^{-1} along with other finger print region signal and all other peaks are good agreement with the proposed structure [8]. The FT-IR spectral data are given in Table 1 and Figure 3.

Table 1: Important IR Bands of Schiff Base with their Assignments

Vibrations	νN-H	ν(ArC-H)	ν(N-N)	ν(C=0)	ν(C=N)
Peak (cm^{-1})	3248	3051	1918	1629	1491

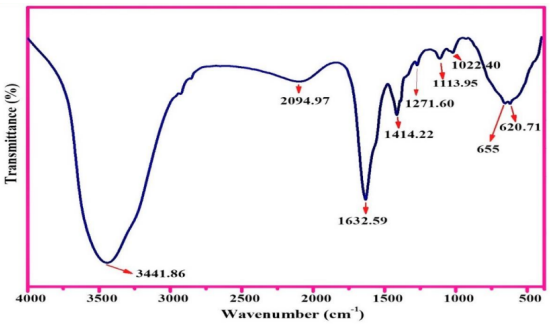

Figure 3: FTIR Spectrum of (E)-N'-(2,4-Dichlorobenzylidene) Nicotinohydrazide

3.2. NMR Studies

In ^{1}H NMR spectrum, the proton attached to C7 & C3 carbon showed as a singlet at δ = 8.99 and 7.78 ppm. The characteristic amine N-H was appeared as broad singlet at δ = 7.65 ppm. On the other hand, the four protons associated with pyridine ring were identified as two doublets at δ = 8.20 & 8.85 ppm, one multiplet at δ = 7.63 ppm and one sharp singlet at δ = 9.27 ppm. In ^{13}C NMR spectrum, the discernible amide carbonyl appeared at δ = 163.2 ppm and it clearly indicates that molecule having amide group on its skeleton. Next, the carbon attached to the adjacent to the nitrogen atom on pyridine ring was appeared at δ = 148.9 and 148.6 ppm. The newly formed imine carbon peak appeared around at δ = 138.7 ppm. The detailed assignments of protons were given in figure 4a,b.

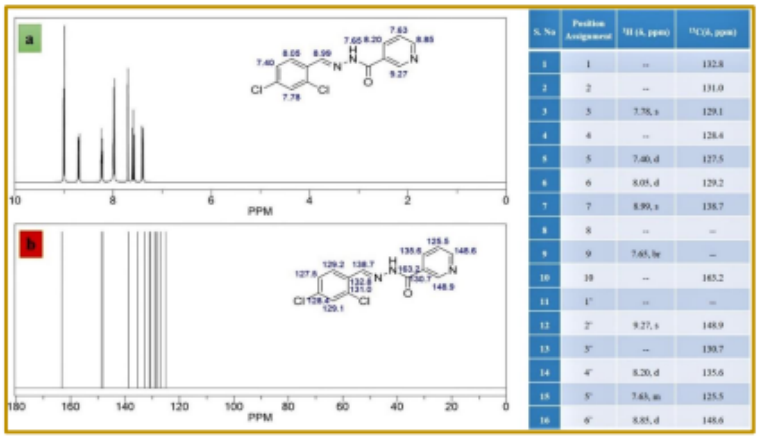

Figure 4: (a) H1 NMR (b) C13 NMR Spectra and Spectroscopic Data (δ) of (E)-N'-(2,4-Dichlorobenzylidene)Nicotinohydrazide

3.3. Solubility and TLC

The crystallized powder tested for solubility and the data given in table 2. Analytical TLC was performed on precoated aluminum sheets of silica (60F254) and visualized by shortwave UV light at λ 254 nm. The compounds are crystallized and tested for solubility among different solvent (plate 2). The TLC plate for (E)-N'-(2,4-dichlorobenzylidene) nicotinohydrazide used single solvent system and tested in polar and non-polar solvents and highly soluble in polar groups.

Table 2: Solubility Test of (E)-N'-(2,4-Dichlorobenzylidene)Nicotinohydrazide

S.No.	Solvents	Room temperature	Hot condition	R_f value
1	Water	Insoluble	Insoluble	–
2	Methanol	Soluble	Soluble	0.90 cm^{-1}
3	Ethanol	Soluble	Soluble	0.73 cm^{-1}
4	Benzene	Soluble	Soluble	0.95 cm^{-1}
5	Hexane	Insoluble	Insoluble	–
6	Chloroform	Soluble	Soluble	0.45 cm^{-1}
7	Dichloromethane	Soluble	Soluble	0.44cm^{-1}
8	Ethyl acetate	Soluble	Soluble	0.95cm^{-1}
9	Dimethyl sulfoxide	Soluble	Soluble	0.93 cm^{-1}

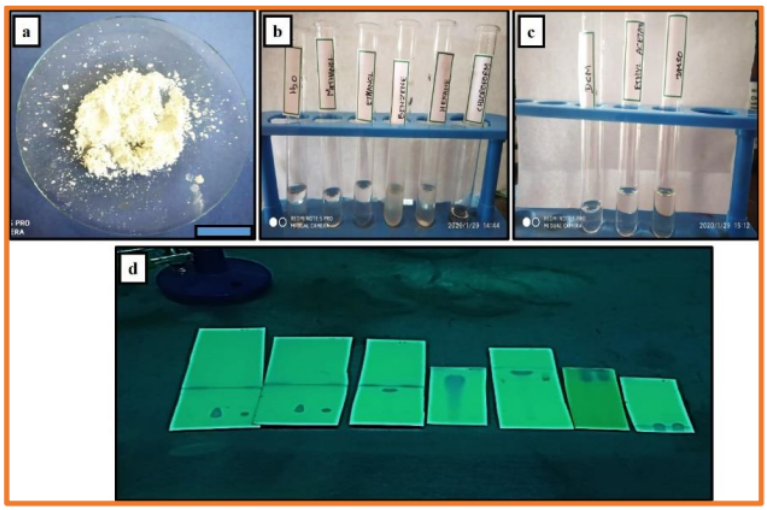

Figure 5: (a) Picture, (b,c) Solubility and (d) TLC Plates of the Synthesized Compound

3.4. Antioxidant Activity

The synthesized compounds exhibited their potent antioxidant properties at 10 μg is more than standard at 20 μg showed 25mM. The ferric ion reducing antioxidant power (FRAP) assay had been designed to measure the antioxidant potential of plasma [9] and was adapted later to evaluate wide range of compounds.

Ascorbic acid	OD	mM
20µg	0.48	25
40µg	1.44	46
60µg	1.73	52
80µg	1.87	60
100µg	1.93	102
Compound (10 µg)	0.51	32

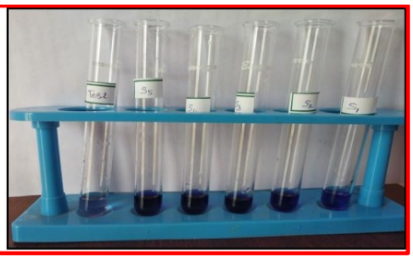

Figure 6: Antioxidant Assay by FRAP Analysis

3.5. Molecular Docking in Silico Study

Binding energy of (E)-N'-(2,4-dichlorobenzylidene) nicotinohydrazide evaluated through molecular docking studies using Glide (in silico analysis). Initially, the structures of these molecules were generated and energy was minimized. Docking studies against caspase revealed that the compound have 3 pose with promising Glide score. The ADME reveals compound is moderately soluble, high GI absorption,

BBB permeant, inhibit cytochrom p family (Table 8). Studies on nicotinohydrazide compounds conducted by Deng et al [10] reported that they have inhibitory activity against caspase-3 and -7. various substituted hydrazones have been reported as anticancer agents by inhibiting nucleic acid synthesis, inhibiti mitosis or induce caspase mediated apoptosis [11].

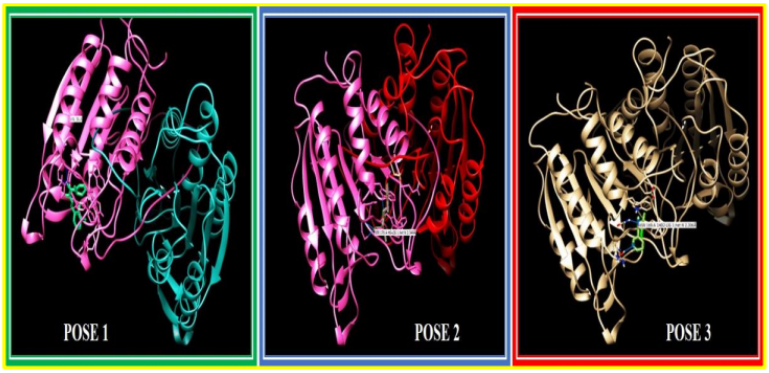

Figure 7: Molecular Docking of (E)-N'-(2,4-Dichlorobenzylidene) Nicotinohydrazide with Caspase 3

Table 3: Docking Score of Ligand with Receptor

Docking score	Aminoacids	Distance of hydrogen bond (Å)
−7	SER170-H LIG O	2.049
	SER170HG LIG	1.955
−6.5	TRP175-LIG N	2.444
	SER170-HLIG N	2.259
	SER170-HG LIG N	2.349
−6.3	ASN169- HLIGN	2.306
	SER170- HLIG N	2.402

3.6. Anticonvulsant Activity

The anticonvulsant activity of the prepared compound was studied by T-maze (Fig.8.A) method using adult zebra fish. The behavioral movement of adult zebrafish in T-maze towards unfavorable and favorable was shown in Table 5. In control, 100% are under favorable environment and scoring 2 with Short bottom swimming. Group II treatment of Pentylenetetrazole (PTZ) induced seizure shows changes in behavior with scoring of 6 due to death of zebrafish. Nearly 80% were survived under unfavourable condition

(Fig.8.b-c), there was a rapid score progression in the first 1h and reached maximum at 3h min period for PTZ. Where as in control group the score ranges 0-1 an ideal experimental condition exhibited spontaneous usual swimming movements consisted by repeated constant short swims. The induced seizure is reverted by Phenytoin within 2h and only 20% moved unfavorable compartment. Similar to positive control PTZ, the prepared compound nicotinohydrazide (Fig.8.e) maintained Short swim and 80% are maintained favourable condition. On the other hand, animals immersed into PTZ solution presented behavioral epileptic seizures, classified in different scores as shown in Table 6. Pentylenetetrazole (PTZ) induced seizure in adult zebrafish clonus-like behavior and have had maximum unfavourable score. The PTZ concentrations induced seizures with score $3 \geq 4 \geq 6$ with in 3h (Table 6). Group 4 PTZ seizure is inverted by Phenytoin within 3 h and the score is $2 \geq 2 \geq 1$ between 0-3 h (Fig.8.d). Similarly the synthesized tested compound nicotinohydrazide has score $2 \geq 0 \geq 0$ between 0-3h and completely reduced the Seizure score 2 to 0 and confirms the antiepileptic drug activity.

Hydrazide/hydrazone derivatives that possess a -CO-NHN=CH- group constitute an important class of compounds for drug development. The specific characteristics of various hydrazide/hydrazone derivatives and structurally related semicarbazones tested as anticonvulsant agents in animals. Aryl acid hydrazones of substituted aromatic acid hydrazides known as nicotinohydrazide was found to be the most potent analog and reported better than that of the prototype drug phenytoin [12].

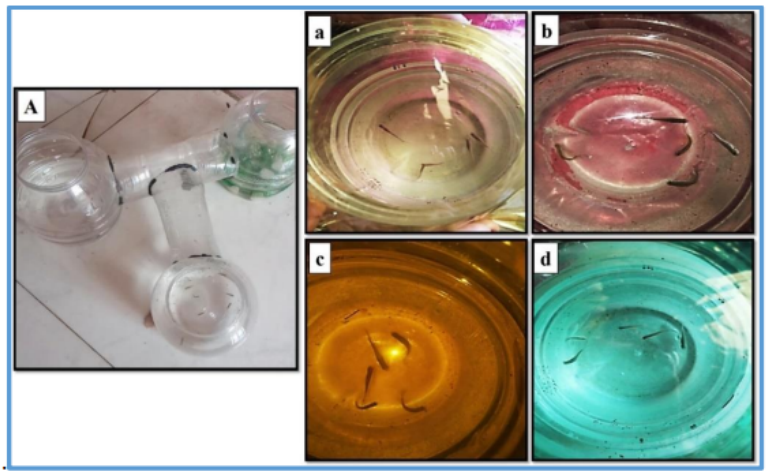

Figure 8: T Maze and Scoring of Zebra Fish induced Seizure. (A) T Maze Experiment, (a) Control, (b) Negative Control, (c) Positive Control, (d) (E)-N'-(2,4-Dichlorobenzylidene) Nicotinohydrazide

Table 4: T-maze Behavior Analysis among Control and Treatment

Groups	Number of Zebra fishes	Favorable Environment	Unfavorable Environment
Group I - Control (Untreated)	7	5	0
Group II- PTZ (Negative control)	7	0	5
Group III - Phenytoin + PTZ	7	4	1

Table 5: T-maze Seizure Score Analysis among Control and Treatment

Group	Event of Behaviour	Scores		
		1h	2h	3h
Group I - Control (untreated)	Short bottom swimming Increased swimming	0	1	1
Group II - PTZ (Negative control)	Circular erratic, clonic movements Fall to the bottom of the tank and dead	3	4	6
Group III - Phenytoin + PTZ	Burst swimming, increaesed swimming and opercula activity	2	2	1
Group IV - MU compound + PTZ	Burst swimming, Increased swimming and Short swim	2	0	0

Score	Behavior Phenotype
0	Short swim mainly in the bottom of the tank
1	Increased activity high frequency of operculaar movement
2	Burst swimming, left and right movements and erratic movements
3	Circular movements
4	Clonic seizure-like behavior (abnormal whole-body rhythmic muscular contraction)
5	Fall to bottom Of the tank, tonic seizure-like (sinking to the bottom of the tank, loss of posture and principally by rigid extension of the body)
6	Death

4. Conclusion

The bioactive aroyl hydrazone (E) N'-(2,4-dichlorobenzylidene) nicotinohydrazide was prepared by Schiff base reaction. The FT-IR, ^{1}H-NMR and ^{13}C- NMR spectral information confirms the successful formation of the prepared compound. This is first time reported that the compound (E) N'-(2,4-dichlorobenzylidene) nicotinohydrazide have had anti antiepileptic drug property. Further, the antioxidant activity confirms that the free radical scavenging activity of nicotinohydrazide was found to be very effective and the docking reveals the compound is potent caspase inhibitors. The *in silico* docking suggest it have anticancer activity. Thus, the prepared compound was found to act as an anticonvulsant and anticancer agent.

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SURVEY OF MEDICINAL PLANTS IN YELAGIRI HILLS AT VELLORE DISTRICT, TAMIL NADU

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Abstract

Ethnobotanical survey has been found to be one of the best approaches to drug discovery. Several active compounds have been discovered from different plants on the basis of ethnobotanical information. During the last few decades, there has been an increasing trend on the study of medicinal plants and their traditional use in different parts of the world. World Health Organization (WHO) has compiled a list of 20,000 medicinal plants used in different part of the globe, 80% of the rural population in developing countries make use of locally available medicinal plants for their primary healthcare needs. About 90% of the country's medicinal plants are found in forest habitats, only 10% of the medicinal plants are distributed surrounded by other landscape sources.

In the present study, ethnobotanical survey was carried out in Yelagiri at Vellore district, Tamilnadu, India. Traditional uses of 150 plant species spread over 44 families are described under this study. The medicinal plants used by them are arranged by scientific name with family name, Vernacular name, Plant parts used and Therapeutic uses. The plants reported in this survey belong to the families such as Acanthaceae, Amaranthaceae, Apiaceae, Apocyanaceae, Asclepiadaceae, Asteraceae, Agavaceae, Cucurbitaceae, Euphorbiaceae, Labiatae, Liliaceae, Malvaceae, Papilionoideae, Verbanaceae, Vitaceae, Solanaceae, Rutaceae, Aristolochiaceae, Alliaceae, Alangiaceae, Annonaceae, Papavaraceae, Moraceae, Basellaceae, Piperaceae, Capparaceae, Caeselpinaceae, Costaceae, Cesalpiniodeae, Lythraceae, Marsileaceae, Poaceae, Sapindaceae, Aizoaceae, Cruciferae, Rubiaceae, Lamiaceae, Bombaceae, Fabaceae and Zingibesaceae. The

present investigation exposed that the medicinal plants still play a vital role in the primary health care of the people.

Keywords: Medicinal Plant, Endangered Species, Forest Habits, Traditional Medicines, Diseases.

1. Introduction

Yelagiri is one of the most famous places for trekkers in India. The hill station is located at a height of 4627.95 feet above sea level. Yelagiri encompasses 14 hamlets and a number of temples spread over several hills. The highest point in Yelagiri is the Swamimalai Hill, standing tall at 4,338 feet; Swamimalai is a destination and viewpoint for trekkers. The hill provides a number of trekking trails through thick reserved forests. Mangalam is a small village, is at the base of this hill. There are other trekking choices that include smaller peaks like Javadi Hills and Palamathi Hills. Yelagiri climate is very cool in Monsoon Season pleasant Weather daily Occurs in This Hill Station classified as tropical. In winter, there is much less rainfall than in summer. Human settlement started 200 to 400 years ago. Most of the native people are 'Vellala caunter' or 'Malayali'. Malayali denotes people who live in mountains. Malayali people also named as "karalar" which means 'one who rules the clouds'. Malayali people statement to come from plains, they are from the Kancheepuram district. The famous Yelagiri Summer festival celebrated in May end is organised by the Tamil Nadu Tourism Development Board. Stalls from different departments, Flowers show, Boat house various cultural programs and Dog Show with a variety of dog breeds are conducted every year. People from all over the State and other parts of the country participate in this annual festival. India is one of the 17 mammoth biodiversity countries in the world. It has 45000 plant species, out of which 15000- 20000 plants have medicinal properties.

In India, plants have been used for medicinal purposes since earliest time, as mentioned in Ayurveda. India is very rich in ethnobotanical heritage. There are over 400 different tribal and other ethnic groups in India. Part of the tribal groups, many other forest dwellers and rural people also possess unique knowledge on plants. The Ethnobotanical studies of different tribal localities may lead to find new information on unexploited natural resources as sources of medicine, food, fodder, fiber, and animal habitat.

Yelagiri is a very rich forested area in terms of plants, Animal and flower diversity which provide many valuable medicinal plants and tribals of the study area are using these plants since ancient time which is yet to record in a proper scientific way. The detailed information on medicinal uses of plants is not available or not recorded well. So the present study suggests that to document all the plant biodiversity resources.

2. Material Methods

Description of Study Area

Yelagiri formally Known as hill station in Vellore district Tamil Nadu 635 853, India Located the latitude for Yelagiri Hills is: 12.579581 and the longitude is: 78.639874 of 1,110.6 metres above Mean Sea Level and spread across 30 km^2. The forest consists of dry mixed deciduous to thorny shrubs with occasional patches of dry evergreen growth. The maximum temperature raises to 44.4°C in May and minimum lies at 11.7°C in January. The average rainfall is about 886 mm.

Vellore District

Yelagiri Hill

Methodology

The study area was surveyed randomly from October 2018 to January 2019. Data was collected from the local People and medicinal practitioners inhabiting the villages of Yelagiri in the Vellore District. In this study, data collection was interviews and detailed personal discussions were conducted with the local people who unique knowledge about the medicinal uses of plants. The discussion contains the details of the plants, parts used, medicinal uses, mode of preparation.

3. Result and Discussion

The Study is based on the survey of traditional information on the medicinal plants from Yelagiri hill of Vellore district. In this study, we focused mainly on plant species documented by the local people in and around the study area for their medicinal uses. Present data are the general results of the ethnobotanical survey conducted from October 2018 to January 2019. Herbal remedies are considered the oldest forms of health care known to mankind on this earth. Earlier to the development of modern medicine, the traditional systems of medicine that has evolved over the centuries within various communities, are still maintained as a great traditional knowledge base in herbal medicines (Mukherjee and Wahil, 2006). Traditionally, this wealth of precious knowledge has been passed on orally from generation to generation without any written document and is still retained by various indigenous groups around the world (Perumal Samy and Ignacimuthu, 2000 and Saranraj et al., 2016). Due to an increasing demand for chemical diversity in screening programs, seeking therapeutic drugs from natural products, interest particularly in ethno medicinal plants has grown throughout the world (Saranraj and Sujitha, 2015). Herbal remedies are considered as the oldest forms of health care known to mankind on this earth. Traditional popular medicine uses the knowledge, skills and practices based on the theories, beliefs and experiences indigenous to its cultures for maintenance of health. Documenting the native knowledge through ethnobotanical studies is important for the conservation and utilization of biological resources. Ethnobotanical survey has been found to be one of the best approaches to drug discovery (Fabricant and Farnsworth, 2001; Kolanjinathan and Saranraj, 2015). In the present study, ethnobotanical survey was carried out in Yelagiri at Vellore district, Tamilnadu, India. Traditional uses of 150 plant species spread over 44 families are described under this study. The tribes and peoples from different rural villages have used the medicinal plants to treat various diseases and disorders like skin allergy, dysentery, antibacterial activity, diabetes, jaundice, asthma, fertility, antifertility, dental diseases, etc. The medicinal plants used by them are arranged by scientific name with Family name, Vernacular name, Plant parts used and Therapeutic uses are furnished in Table-1. The plants reported in this survey belong to the families such as Acanthaceae, Amaranthaceae, Apiaceae, Apocyanaceae, Asclepiadaceae, Asteraceae, Agavaceae, Cucurbitaceae, Euphorbiaceae, Labiatae, Liliaceae, Malvaceae, Papilionoideae, Verbanaceae, Vitaceae, Solanaceae, Rutaceae, Aristolochiaceae, Alliaceae, Alangiaceae, Annonaceae, Papavaraceae, Moraceae, Basellaceae, Piperaceae, Capparaceae, Caeselpinaceae, Costaceae, Cesalpiniodeae, Lythraceae, Marsileaceae, Poaceae, Sapindaceae, Aizoaceae, Cruciferae, Rubiaceae, Lamiaceae, Bombaceae, Fabaceae and Zingibesaceae.

In India, there are about 54 million indigenous people of various ethnic groups inhabiting various terrains. These indigenous groups possess their specific distinct culture, religious rites, food habit and have a rich knowledge of traditional medicine.

Even today, indigenous and certain native communities practiced herbal medicine to cure a variety of diseases, with plants particularly used as folk medicine to treat snakebites (Parinitha et al., 2005). Utilization of plants for medicinal purposes in India has been reported long back in ancient literature because they are essential to human survival (Mohamed Tariq and Md Rayees Ifham, 2013; Sastri et al., 1996). The consumption, management and valuation of wild plants are central aspects of the traditional knowledge in many human populations. Thus, plants gathering, the diffusion and conservation of knowledge within the community are traditional practices that have contribution to the subsistence of many cultures. In most of the societies the medical system co-occurs with several traditional systems. These traditional medical systems are generally based on the uses of natural and local products which are commonly related to the people's perspective on the world and life (Toledo et al., 2009). In this study, a botanical survey was carried out in Vellore district, Tamilnadu, India. Traditional uses of 150 plant species spread over 44 families are described under this study. The tribes have used the plants to treat skin allergy, dysentery, anti-bacterial activity, diabetes, jaundice, asthma, fertility, antifertility, dental diseases, etc. The medicinal plants used by them are arranged alphabetically followed by family name, local name and medicinal uses.

Table 1: List of Medicinal Plants in Yelagiri Hills at Vellore District

S.No	Plant Name	Local Name	Parts Used	Therapeutic Use
1	*Adhatoda vasica* (Acanthaceae)	Adathodai	Aerial parts	Bronchitis, Leprosy, Heart troubles, Asthma, Cough, Sore eyes and Gonorrhea
2	*Andrographis Paniculata* (Acanthaceae)	Seriyanangai or Nilavembu	Leaf	Snake bites and Liver diseases
3	*Alternanthera sessilis* (Amaranthaceae)	Ponnakanni	Leaf	Burning sensation, Diarrhoea, Leprosy, Skin diseases and Fever
4	*Amaranthus Graecizans* (Amaranthaceae)	Serukeerai	Aerial parts	Antimicrobial activity
5	*Amaranthus spinosus* (Amaranthaceae)	Mullikkirai	Leaf	Leprosy, Eczema, Nausea, Fever and Anaemia
6	*Achyranthes aspera* (Amaranthaceae)	Naivooruvi	Leaf	Wounds
7	*Amaranthus artis* (Amaranthaceae)	Araikeerai	Leaf	Antimicrobial activity

8	*Amaranthus viridis* (Amaranthaceae)	Kuppaikeerai	Leaf	Antimicrobial activity
9	*Amaranthus blitum* (Amaranthaceae)	Mulaikeerai	Leaf	Antimicrobial activity
10	*Amaranthus spinosus* (Amaranthaceae)	Mullikeerai	Leaf	Antimicrobial activity
11	*Acalypha indica* (Euphorbiaceae)	Kuppaimeni	Leaf	Leaf juice is applied externally for curing body itching
12	*Aloe vera* (Liliaceae)	Kathazai	Aerial parts	Promotes menstrual flow, Heals wounds and fresh cuts, Eye diseases, Asthma, Leprosy and Jaundice
13	*Abutilon indicum* (Malvaceae)	Thuthi	Leaf	Antimicrobial activity
14	*Azadirachta indica* (Meliaceae)	Veempu (Neem)	Leaf	Powdered leaves are used for diabetes
15	*Aegle marmelos* (Rutaceae)	Vilvam	Leaf	The dried and powdered leaves are used for diabetes
16	*Aristolochia bracteolate* (Aristolochiaceae)	Aaduthinnappalai	Leaf	Leaf juice is taken orally to treatment of diabetes
17	*Allium sativum* (Lilliceae)	Vellai poondu	Leaf	Juices of the leaves is used for diabetes
18	*Allium cepa* (Alliaceae)	Vengkaayam	Bulb onion	Bulb of the onion is used for diabetes
19	*Alangium salvifolium* (Alangiaceae)	Alengi	Aerial part	Antioxidant and antimicrobial activities
20	*Aerva lanata* (Acanthaceae)	Sirupolai	Aerial part	Leaf juice applied externally on bitten area and applied externally to cure chronic wounds
21	*Annona squamosal* (Annonaceae)	Setha	Fruits	Intestinal worms

22	*Anisomeles malabarica* (Labiatae)	Peruntumpai	Aerial part	The plant is useful halitosis, amentia, intestinal worms and fever arising from teething in children
23	*Amaranthus virudis L.* (Amaranthaceae)	Thoia	Leaf	Leaf paste is applied over the infected area to cure erysipelas
24	*Argemone mexicana Linn.* (Papavaraceae)	Braman thandu	Latex	Latex applied on infected parts to cure ringworm infection
25	*Artocarpus hirsutus Lam.* (Moraceae)	Kattupala	Fruit	Fruits used as appetizer, seed with honey used to treat asthma
26	*Basella alba* (Basellaceae)	Kodipasalai	Leaf	Antimicrobial and Anticancer activity
27	*Brassica juncea* (Cruciferae)	Kaduku	Leaf Seeds	Eye diseases
28	*Betel piper Linn* (Piperaceae)	Vetrilai	Leaf	Leaves vermifuge, antiseptic, anti-diabetics, astringent, antiperiodic
29	*Cleome gynandra* (Capparaceae)	Nalvelai	Leaf	Toothache
30	*Cichorium intybus* (Asteraceae)	Kasinikeerai	Leaf	Antimicrobial activity
31	*Calotropis gigantean* (Asclepiadaceae)	Erukkam	Leaf Milk	Cure rheumatic Joints pain and swellings
32	*Coccinia grandis* (Cucurbitaceae)	Kovai	Leaf	Eye diseases
33	*Cucumis sativus* (Cucurbitaceae)	Vellari	Leaf Fruits	Fever, Bronchitis, Jaundice, Haemorrphages Strangury and General debility
34	*Cassia auriculata* (Caesalpinacea)	Avaram	Flower	Daily three or four flower are taken regularly
35	*Cajanus cajan* (Fabaceae)	Thovaray	Seed	Seeds boiled and taken along with food items

36	*Costus igneus* (Costaceae)	Kostum	Leaves	Leaves juice is used for the treatment of diabetes
37	*Colocasia esculenta* (Araceae)	Shaeppamkizhangu	Leaves	Powdered leaves are used to treat diabetes
38	*Curcuma longa* (Zingiberaceae)	Kasturimanjal	Rhizome	Rhizome is used for diabetes
39	*Celosia argentea* (Amaranthaceae)	Pannaikeerai	Leaf	Antimicrobial activity
40	*Centella asiatica* (Apiaceae)	Vallari	Aerial parts	Antimicrobial activity and Increase the memory power
41	*Coriandrum sativum* (Apiaceae)	Kothamalli	Leaf	Antimicrobial activity
42	*Catharanthus roseus* (Apocyanaceae)	Nithyakalyani	Aerial parts	Antimicrobial and Anticancer activity
43	*Clitoria ternatea* (Fabaceae)	Sangu Pushpam	Leaf	Antimicrobial activity, Eye diseases and Headache
44	*Ceiba pentandra* (Bombacaceae)	Ilavam	Aerial part	Diuretic, antipyretic, tonic, gonorrhoea, dysuria, acrid, bitter, thermogenic febrifuge, emetic tonic and tumours
45	*Cassia tora* (Cesalpinioideae)	Tagarai	Aerial part	Malaria, ring worm, chronic inflammation of the skin and other skin diseases
46	*Caesalpinia bonduc* (Cesalpinioideae)	Kaccakkay	Aerial part	Fever, cough, worms, flatulence, dyspepsia, jaundice, arthritis, splenomegaly and diabetes
47	*Cassia fistula* (Cesalpinioideae)	Sarakondrai, Konnei	Aerial part	Bark decoction mixed with garlic and powdered pepper is given to cattle as purgative
48	*Cassia alata* (Cesalpinioideae)	Seemaiakathi	Leaf	Ringworm patches, cough and eczema

49	*Cassia roxburghii* (Cesalpinioideae)	Sennkondrai	Leaf	Hepatoprotective activity
50	*Cassia obtuse* (Cesalpinioideae)	Nilaavarai	Leaf	Antimicrobial activity
51	*Crateva adansonii* (Capparaceae)	Mavelangam	Leaf	Fever, acrid and cough
52	*Carica papaya* (Caricaceae)	Pappali	Leaf, fruits	Tuberculosis and promotes menstrual flow
53	*Citrus limon (Linn.) Burm* (Rutaceae)	Elumichai	Fruit	Fruit is used to cure nail infection, juice induces freshness to body
54	*Cucurbita moschata* (Cucurbitaceae)	Poosani	Leaf and Fruits	Burns, Scalds, Inflammations, Abscesses, Boils, Migraine and Neuralgia
55	*Cynodon dactylon* (Poaceae)	Arugampul	Whole parts	Antimicrobial and Diabetes
56	*Cardiospermum halicacabum* (Sapindaceae)	Mudakkaththan	Leaf	Rheumatic arthritis
57	*Cissus quadrangularis* (Vitaceae)	Perandai	Aerial Parts	Heart diseases, diabetes and metabolic Syndrome
58	*Datura metel* (Solanaceae)	Vellaiumattai	All parts	Antimicrobial and Anticancer activity
59	*Datura stramonium* (Solanaceae)	Umattai	All parts	Antimicrobial and Anticancer activity
60	*Erythrina indica Lam.* (Fabaceae)	Kalyana murungai	Leaf	Leaves relive body pain; headache, fever, cold, fruits treat diabetics
61	*Eucalyptus globules Labill.* (Myrtaceae)	Neelagri	Leaf	Latex is applied on the skin to alleviate body pain & never disorders
62	*Euphorbia hirta* (Euphorbiaceae)	Amman pacharisi	Leaf	Leaf juice is taken orally for treatment of diabetes

63	*Eclipta alba* (Asteraceae)	Karsalamkanni	Leaf	Leaf is used for the treatment of Diabetes
64	*Enicostemma littorale* (Gentianaceae)	Vellaruku	Leaf	The powered leaves are used for diabetes
65	*Ervatamia divaricate* (Apocyanaceae)	Nantiyavarttam	Leaf	Antibacterial and Antifungal activity
66	*Eugenia jambolana* (Myrtaceae)	Naval	Seed	Early morning seeded powered is taken to cure diabetes
67	*Euphorbia heterophylla* (Euphorbiaceae)	Amman Paccarici	Aerial parts	Remove intestinal worms
69	*Eclipta prostrate* (Asteraceae)	Karisalankanni	Whole parts	Antibacterial activity and Eye diseases
70	*Eclipta procera* (Asteraceae)	Mangel Karisalankanni	Whole parts	Antibacterial activity and Jaundice
71	*Furcraea foetida* (Agavaceae)	Annaikatraiei	Leaf	Anti-inflammatory and wound healing
72	*Ficus racemosa* (Moraceae)	Atthi	Root	Root decoction is taken orally to cure diabetes
73	*Ficus benghalensis* (Moraceae)	Aalamaram	Bark	Bark decoction is used for diabetes
74	*Ficus religiosa* (Moraceae)	Arasu	Leaf	Antibacterial activity
75	*Gisekia pharnaceoides* (Aizoaceae)	Manalikkirai	Aerial parts	Antibacterial activity
76	*Gymnema sylvestre* (Apocyanaceae)	Sakkaraikolli	Leaf	Leaf juice is taken daily
77	*Hemidesmus Indicus* (Asclepiadaceae)	Nannari	Aerial parts	Fever and Skin diseases
78	*Hygrophila auriculata* (Acanthaceae)	Nirmulli	Leaf and Seed	Used against cough, seeds used as aphrodisiac and increase male fertility
79	*Hibiscus rosasinensis* (Malvaceae)	Semparuthi	Leaf	Flower Hair growth and hair infections

80	*Hibiscus cannabinus* (Malvaceae)	Pulichakeerai	Leaf	Antimicrobial activity
81	*Ipomoea batatas (Linn.)* (Convolvulaceae, Moraceae)	Sakaraivalli	Tubers	Tubers boiled and taken to treat diabetics
82	*Ixora coccinea* (Rubiaceae)	Idlipoo	Leaf Flower	Liver toxicity
83	*Justicia Tranquebariensis* (Acanthaceae)	Sivanarvembu	Leaf	Swelling and snake bites
84	*Jatropha gossypifolia* (Euphorbiaceae)	Kadal amanakku	Entire plant	Toothache and angular stomatitis, plant latex is used to cure Headache
85	*Lantana camara Linn* (Verbenaceae)	Unni chedi	Leaf	Leaf juice improves digestion in children and fruits - treat diabetics
86	*Lucas aspera Sprong* (Lamiaceae)	Thumbai	Leaf	Leaves used to relive tooth ache and prevents tooth/gum infection
87	*Lagenaria siceraria* (Cucurbitaceae)	Sorakkai	Leaf	Cough, Bronchitis, Asthma, Fever, Inflammations, Leprosy, Skin diseases, Jaundice, Decaying teeth, Flatulence and Baldness
88	*Lactuca sativa* (Asteraceae)	Manalikeerai	Leaf	Antimicrobial activity
89	*Lablab purpureus* (Papilionoideae)	Avarai	Leaf	Alexipharmic, Emmenagogue, Astringent, diuretic, anaphrodisiac, stomachic and antispasmodic

90	*Lawsonia inermis* (Lythraceae)	Maruthani	Leaf	Antimicrobial activity and Cooling of body. Leaves applied on foot to cure etching and healing of the crack
91	*Leucas aspera* (Labiatae)	Thumbai	Leaf	Leaf juice is given with honey to treat bronchitis in children
92	*Mentha arvenis* (Lamiaceae)	Pudhina	Leaf	Antimicrobial activity
93	*Morinda coreia* (Rubiaceae)	Nuna	Leaf	Antibacterial activity
94	*Murrya koeingii* (Rutaceae)	Karuvepalai	Leaf	Leaf juice is taken to treat diabetes
95	*Moringa oleifera* (Moringaceae)	Murungai	Leaf	Early morning leaf juice is taken orally to cure diabetes
96	*Mangifera indica* (Anacardiaceae)	Mamaran	Leaf	The powered leaves are mixed with cow milk and taken orally to cure diabetes
97	*Melia azedarach* (Meliaceae)	Malai vembu	Seed	Seeds is used for the treatment of diabetes
98	*Marsilea minuta* (Marsileaceae)	Aarakkerai	Leaf	Antimicrobial and Diabetes
99	*Mollugo cerviana* (Aizoaceae)	Porpadakam	Aerial part	Treat fever
100	*Musa paradisiaca* (Musaceae)	Valai, tatam	Stem	Juice is obtained from pseudostem is taken orally to dissolve the Kidney stone
101	*Murraya koenigii* (Rutaceae)	Kariveppilai	Leaf	Dysentery, blood purifier, tuberculosis and burning pain

102	*Mukia maderaspatana* (Cucurbitaceae)	Musumusukai	Leaf	Burning sensation, Dipsia, Flatulence, Colic consumption, Ulcers, Cough, Asthma, Neuralgia, Notalgia, Odontalgia and Vertigo
103	*Momordica somnifera* (Cucurbitaceae)	Pavakai	Leaf and Vegetable	Antimicrobial, Antioxidant and Antidiabetic activity
104	*Melochia corchorifolia* (Malvaceae)	Pinnakukeerai	Leaf	Antimicrobial activity
105	*Mimosa pudica* (Mimosaceae)	Thottasurungi	Leaf	Wounds
106	*Nelumbo nucifera Gaertn* (Nymphiaceae)	Alli	Flower	Flowers made to juice and taken to treat diabetics
107	*Ocimum sanctum* (Labiatae)	Thulasi	Leaf	Leaf juice is mixed with cumin is given to cure the dry cough
108	*Ocimum basilicum* (Labiatae)	Karpura Thulasi	Leaf	Leaf juice is mixed with cumin is given to cure the ear pains
109	*Oxalis corniculata* (Oxalidaceae)	Pulichcha keerai	Leaf	Antimicrobial activity
110	*Piper nigrum L* (Piperaceae)	Milagu	Fruit	Seeds taken orally to reduce throat infection, cold and cough
111	*Plumeria obtuse L* (Apocynaceae)	Thevarali	Latex	Latex is used as a mouth wash, and used to cure mouth ulcer
112	*Pistia stragiotes* (Araceae)	Akayattamarai	Aerial parts	Bladder complaints, Kidney afflictions, Diabetes, Hematuria, Dysentery and Anemia
113	*Plectranthus amboinicus* (Lamiaceae)	Karpuravalli	Leaf	Antimicrobial activity

114	*Portulaca oleraceae* (Portulaceae)	Paruppukeerai	Leaf	Antimicrobial activity
115	*Portulaca quadrifida* (Portulaceae)	Mukulikeerai	Leaf	Antimicrobial activity
116	*Punica granatum* (Lythraceae)	Madulai	Flower	Flower is very good antidiabetic properties
117	*Phyllanthus amaru* (Euphorbiaceae)	Kilanelli	Leaf	Leaf juice is taken orally to treat diabetes
118	*Phyllanthus emblica* (Euphorbiaceae)	Nellikkaai	Fruit	Fruits are very good antioxidant properties
119	*Psidium guajava* (Myrtaceae)	Koiyaa	Fruit	Daily one fruits is taken to cure diabetes
120	*Polyalthia longifolia* (Annonaceae)	Nettilinkam	Leaf	Fever, gonorrhea, uterus aliment, leucorrhoea, mouth ulcer heart problem, blood pressure and stimulated respiration
121	*Pterocarpus marsupium* (Papilionoideae)	Vengai	Aerial part	Astringent, bitter, acrid, cooling, anti- inflammatory union- promoter, depurative, urinary astringent, alterant, rejuvenating. Leprosy, fractures, skin diseases, diabetes cough, asthma and graying hair
122	*Plumeria rubra* (Apocyanaceae)	Segappu Arali	Leaf	Ulcers, Pruritus, Leprosy
123	*Pergularia daemia* (Asclepiadaceae)	Uttamani	Leaf	Bath with leaf decoction is taken to cure body pain
124	*Rhinacanthus nasutus* (Acanthaceae)	Nagamalli	Leaf	Leaves boiled with gingelly oil are applied to treat toothache
125	*Ricinus communis* (Euphorbiaceae)	Amanakku	Seed	Seed oil is used for cooling the body during fever

126	*Sesbania grandiflora* (Papilionoideae)	Agathei	Leaf	Cooked leaves are taken to get cooling effect to infected eyes
127	*Spinacea oleracea* (Amaranthaceae)	Palakeerai	Leaf	Antimicrobial activity
128	*Solanum trilobatum* (Solanaceae)	Thuthulai	Leaf	Antimicrobial activity and Cough
129	*Solanum nigrum* (Solanaceae)	Manathakalli	Aerial parts	Antimicrobial activity
130	*Solanum torvum* (Solanaceae)	Sundai	Aerial parts	Skin diseases, Inflammations, Colic, Flatulence, Rheumatoid arthritis, Cough, Fever, Asthma, Bronchitis, Urinary retention and Kidney stones
131	*Spermacoce hispida* (Rubiaceae)	Nathachuri	Leaf	The powered leaves are taken twice daily
132	*Syzygium cumini (L.) Skeels* (Myrtaceae)	Naval Palama	Seed	Seed powdered and used to treat diabetics and reduce the level of sugar in the blood
133	*Tribulus lanuginosis L.* (Zygophylaceae)	Nerungi	Fruit	Seed powder used to increase fertility and sperm production
134	*Typhonium trilobatum* (Araceae)	Karunai	All parts	Antibacterial activity
135	*Trigonella faenum* (Fabaceae)	Vendhayakeerai	Leaf	Antimicrobial activity
136	*Tamarindus indica* (Cesalpinioideae)	Puli	Fruit	Fresh fruit pulp paste mixed with lime is applied on the painful muscle swelling
137	*Tridax procumbens* (Rubiaceae)	Kenatrupasan Vettukaya puntu	Leaf	Leaf juice is applied externally for healing wounds

138	*Thespesia populnea* (Malvaceae)	Puvaracu	Leaf	Skin disease
139	*Tinospora cordifolia* (Menispermacee)	Seenthil	Leaf	Treat piles
140	*Vinca rosea* (Apocynaceae)	Nittiyakalyani	Leaf	Leaf juice is taken orally to treat diabetes
141	*Vigna mungo* (Papilionoideae)	Oolunthu	Aerial part	Rheumatism, Nervous diseases, Liver diseases, Diuretic, Dropsy and Cephalalgia
142	*Vitex negundo* (Verbanaceae)	Nochi	Leaf	Headache and Sinus problem
143	*Withania somnifera* (Solanaceae)	Ashwagandha	All parts	Antimicrobial activity and Leaf paste in cow's milk used to treat asthma
144	*Nerium oleander (sol)* (Apocynaceae)	Arali	Fruit Edible	Ear pain
145	*asparagus racemosus (Roxb)* (Liliaceae)	Thaneervitan Kizhangu	Root	Stomach(dyspepsia), constipation, stomach spasms, and stomach ulcers
146	*Blepharis medaraspatensis (L)* (Acanthaceae)	Elumbu otti	Seeds	dysuria, diseases of nervous system, diuretic, aphrodisiac
147	*Hyptis suaveolens Linn* (Lamiaceae)	Kattutulsi	Root decoction	Appetizer Fabaceae
148	*Millettia pinnata* (Fabaceae)	Punga maram	Flowers	anti-diabetic action
149	*Premna integrifolia Linn* (Verbanceae)	Mullai	Root, leaves, Bark	Neuralgia, Arthritis, Common cold
150	*Jasminum angustifolium* (Oleaceae)	Kattu Malligai	Root and flower	Skin diseases, ulcers, diseases of eye, stomatitis, pruritus, anti-toxic

4. Conclusion

The survey reveals that Yelagiri hill is enriched with many plants. The medicinal plants in the hill are still used by the local inhabitants for many purposes. The biodiversity of the hill should be further explored and conserved in future. Through this ethnobotanical survey, the availability and presence of many medicinal plants have been investigated and verified. We observed that these plants are be used as drugs by pharmacologically unexplored areas of India, which may be utilized for the better human health. This study offers a model for studying the relationship between plants and people, within the context of traditional remedies. This study also gathered a broad spectrum of information concerning medicinal plants used by the peoples of Vellore district. The survey shoews that, the study area has outstanding plant diversity with plenty of medicinal plants to treat a wide spectrum of human ailments. It is evident from the interviews conducted in different villages such as Attanaoor, Nilaoor, Mangalam etc. knowledge of medicinal plants is limited to traditional healers, herbalists who are living in rural areas and collecting the medicinal plants from the Yelagiri unscientifically. It is concluded that the unscientific collection of ethnobotanical plants from the Yelagiri of Vellore district possess greater pressure on the depletion of diversity of the local region. Hence, there is an urgent need to assess the biodiversity of the local forest, and conserve the biodiversity as well as the traditional knowledge by proper documentation and conservation strategies.

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Part B:

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RESEARCH TRENDS IN INDIA IN THE FIELD OF CRYSTALLOGRAPHY WITH REFERENCE TO WEB OF SCIENCES 2009 – 2018

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Abstract

This paper analysis to highlight the growth and development of Crystallography literature in India and make the quantitative and qualitative assessment of research output based on web of Science database. A total of 2030 publication were published in India on Crystallography, which received 25129 citations during 2009-2018. The average number of publications per year was 203 and the average number of citation per publication was 135.51. The publication peaked in 2017 with 262 and the highest number of citations of 3793 was received in 2014.In the international level India stood in 6th position in Crystallography literature publication. All 100% of the publications referred for this appeared in English language. The Web of Science database was used for retrieving data on Crystallography during 2009-2018, using search term namely "Crystallography" in topic field. A total of 2030 publications and citations 25129 received to these publications were downloaded and transferred to spread sheet publications. The bibliographic fields were analyzed by normal count procedure for countries, authorship, journals, research areas and language etc. A total of 2030 publications were published during 2009-2018, which received 25,129 citations during the period. There were 151 publication in 2009 on Crystallography. Year wise distribution of publication and growth rate of publication have been tabulated in this paper. The highest number of publication 262 was in 2017. The highest number of citation of 3793 was in the year 2014. The average number of publications per year was 203 and the number of citations per publication during the period was 135.51. The highest annual growth rate 55.86 was analyzed in 2014. Year wise growth rate of publications and citations on crystallography has been analyseds. The highest number of citation per publication 38.23 was in 2016. The fluctuation trend in growth of publications was viewed in this study.The study finds India at the 6th position with regard to the research Publications in Crystallography.

Keywords: Scientomertics, Crystallography, Relative Growth Rate (RGR) and Doubling Time (DT) of Publication.

1. Introduction

Crystallography is a branch of science that deals with discerning the arrangement and bonding of atoms in crystalline solids and with the geometric structure of crystal lattices. Classically, the optical properties of crystals were of value in mineralogy and chemistry for the identification of substances. Modern crystallography is largely based on the analysis of the diffraction of X-rays by crystals acting as optical gratings. Using X-ray crystallography, chemists are able to determine the internal structures and bonding arrangements of minerals and molecules, including the structures of large complex molecules, such as proteins and DNA.

2. Literature Review

Neelamma & Gavisiddappa Bhalappa Anandhalli (2015) [3] made a study which revealed thevarious aspects of crystallography literature such as year wise distribution, relative growth rate, doubling time of the literature, geographical wise, organizations wise, Languagewise, form wise, most prolific authors etc. The highest number of articles was published in the year 2011, while lowest numbers of research articles were reported in the year 1999. Further the relative growth rate is gradually increased and on the other hand doubling time decreased.

Santhakumar (2018) [4] made an attempt to highlight the publication status and growth of global cosmic rays research publication output of Web of Science during 2004-2013. A total of 20395 publications were published on cosmic rays during this period. The average number of publications per year is 2039.5 and the highest numbers of publications 2565 were published in 2009. Out of total publications, 5288 were produced by mega authors and2794 by multi authors. Pattern of Co-Authorship revealed that the improving trend of co-authored publications. The average value of Collaboration Coefficient for cosmic rays is 0.64.

Hemalatha & Thiruvengada Mani(2019) [1] analyzed to highlight the growth and development of Psychological Science literature and make the quantitative and qualitative assessment of research output based on web of Science database. A total of 8057 publication were published on Psychological Science, which received 103377 citations during 2009-2018. The average number of publications per year 805.7 and the average number of citations per publication was 15.44. The publication peaked in 2017 with 1293 and the highest number of citations of 2005 was received in 2018. USA had the highest share 2955 (36.68%) of publications and citation 60801 (58.81%) followed by England with 874 (10.84%) publications and 20695 (20.01%) citations. Netherland had the highest Publication Efficiency Index (292.84%) followed by England with (184.54%). More than 89% of the publications appeared in English language (89.32%).

3. Objectives

The Objective of the study is to perform a Scientometrics analysis of all Crystallography research publications in India. The parameters of the study focus on the following aspects:

- To depict the growth rate of publication and citations
- Relative growth rate (RGR) and Doubling Time(DT) of publication
- To examine the authorship pattern of publication
- Pattern of Co-Authorship indexes CAI
- Most prolific authors
- Highly preferred journals
- Language wise distribution of publications
- Research areas wise distribution of publication output
- To find out the most preferred source titles.

4. Materials and Methods

The Web of Science database was used for retrieving data on Crystallography during 2009-2018, using search term namely "Crystallography" in topic field. A total of 2030 publications and citations 25129 received to these publications were downloaded and transferred to spread sheet publications. The bibliographic fields were analyzed by normal count procedure for countries, authorship, journals, research areas and language etc.

5. Results and Discussions

5.1. Forms of Publications

Table 1 reveals that the major source of publication covered by web of science database on crystallography research is Research Articles with 1978 Publications (96.45%) followed by Reviews with 52 Publications (2.56%). Proceedings Paper 15 Publications (0.73%). The result indicates that the research outputs on the subject of the period covered by the study are mostly published in the form of Research Articles in Journals.

Table 1: Forms of Publications

Sl. No.	Document Types	No. of Publications	%
1	Research Article	1958	96.45%
2	Review	52	2.56%
3	Proceedings Paper	15	0.73%
4	Editorial Material	13	0.64%
5	Book Chapter	6	0.29%
6	Letter	7	0.19%
7	Meeting Abstract	2	0.09%

5.2. Year wise Growth Rate of Publications and citations

Annual Growth Rate (AGR) of Publications

Table 2 provides the AGR of the number of documents for period 2009 to 2018.

$$\frac{\text{End Value - First Value AGR}}{\text{First Value}} \times 100$$

A total of 2030 publications were published during 2009-2018, which received 25,129 citations during the period. There were 151 publication in 2009 on Crystallography. Year wise distribution of publication and growth rate of publication is given in table 2. The highest number of publication 262 was in 2017. The highest number of citation of 3793 was in the year 2014. The average number of publications per year was 203 and the number of citations per publication during the period was 135.51. The highest annual growth rate 55.86 was analyzed in 2014. Table 1 provides year wise growth rate of publications and citations on crystallography. The highest number of citation per publication 38.23 was in 2016. The fluctuation trend in growth of publications was viewed in this study.

Table 2: Year Wise Growth of Publications and Citations

Sl. No.	Year	No of publication	Percentage of TP	Growth Rate of Publication	No. of citations	Percentage of TC	CPP	Growth Rate of Citations
1	2009	151	7.43	–	3477	13.83	23.02	–
2	2010	135	6.65	-10.59	2806	11.16	20.78	-19.29
3	2011	147	7.24	8.88	2644	10.52	17.98	-5.77
4	2012	177	8.71	20.40	3193	12.70	18.03	20.76

5	2013	179	8.81	1.12	3064	12.19	17.11	-4.04
6	2014	279	13.74	55.86	3793	15.09	13.59	23.79
7	2015	251	12.36	-10.03	2874	11.43	11.45	-24.22
8	2016	236	11.62	-7.96	1775	7.06	7.52	38.23
9	2017	262	12.90	11.01	1155	4.59	4.40	-34.92
10	2018	213	10.49	-18.70	348	1.38	1.63	-69.87
	Total	2030	100.00	–	25129	100.00	135.51	–

TP= Total Publication, TC = Total citations, CPP= Citations per Publication

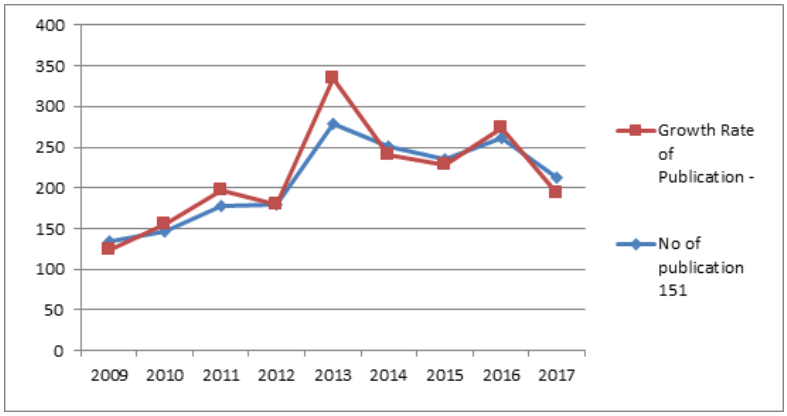

Figure 1: Relative Growth Rate (RGR) and Doubling Time (DT) of Publication

The Relative growth rate (RGR) is the increase in number of articles or pages per unit of time. This definition derived from the definition of relative growth rates in the study of growth analysis in the field of mobile technology. The mean relative growth rate (R) over the specific period of interval can be calculated from the following equation.

Relative growth rate (RGR)

$$1 - 2R = LogW2LogW1/T2 - T1$$

where

1-2 R - mean relative growth rate over the specific period of interval
Loge W1 - log of initial number of articles
Loge W2 - log of final number of articles after a specific period of interval
T2-T1 - the unit difference between the initial time and the final time.

The year can be taken here as the unit of time.

$$\text{Doubling Time (DT)} = 0.693/R.$$

Table 3: Relative growth rate (RGR) and Doubling Time (DT) of Publication

Year	No. of Publication	Cumulative Total	W1	W2	RGR	DT
2009	151	–	–	5.01	–	–
2010	135	286	5.01	4.90	-0.11	-6.3
2011	147	433	4.90	4.99	0.09	7.7
2012	177	610	4.99	5.17	0.18	3.85
2013	179	789	5.17	5.18	0.01	69.3
2014	279	1068	5.18	5.63	0.45	1.54
2015	251	1319	5.63	5.52	- 0.11	- 6.3
2016	236	1555	5.52	5.46	- 0.06	- 11.55
2017	262	1817	5.46	5.56	0.1	6.93
2018	213	2030	5.56	5.36	- 0.2	3.46

Table 4: Highly Productive Countries

Rank	Country	Total Publication	Total Citations	CPP
1	USA	8694 (28.92%)	223535	25.71
2	Peoples R china	4517 (15.02%)	57429	12.71
3	Germany	3464 (11.52%)	82496	23.81
4	England	2942 (9.78%)	102897	34.97
5	Japan	2327 (7.74%)	38869	16.70
6	India	2030 (6.75%)	25129	12.37
7	France	1966 (6.54%)	37343	18.99
8	Canada	1184 (3.93%)	21172	17.88
9	Australia	1106 (3.67%)	17832	16.12
10	Italy	1061(3.53%)	18122	17.08

Highly productive Countries

Table 3 above shows the Relative Growth Rate (RGR) and Doubling Time (DT) of Publications. Table 4 above was included in the paper to show that India stands in 6th position in the International Publications of Crystallography Research.

Table 5: Authorship Pattern of Publication

Year	Single	Two	Three	Four	Five	Six	Seven	Eight	Nine	Ten	>Ten	Total Paper
2009	6 (9.5%)	9 (4.4%)	30 (8.5%)	36 (9.1%)	38 (10.8%)	17 (6.4%)	5 (2.9%)	4 (4.7%)	1 (2.1%)	1 (2.5%)	4 (5.7%)	151
2010	5 (7.9%)	11 (5.4%)	26 (7.3%)	41 (10.4%)	21 (6%)	15 (5.7%)	10 (5.9%)	2 (2.3%)	1 (2.1%)	1 (2.5%)	2 (2.8%)	135
2011	0	20 (9.9%)	29 (8.2%)	26 (6.6%)	33 (9.4%)	19 (7.2%)	7 (4.1%)	6 (7%)	3 (6.3%)	2 (5.1%)	2 (2.8%)	147
2012	3 (4.7%)	16 (7.9%)	31 (8.8%)	39 (9.9%)	42 (12%)	19 (7.2%)	12 (7.1%)	9 (10.5%)	4 (8.5%)	1 (2.5%)	1 (1.4%)	177
2013	6 (9.5%)	27 (13.4%)	24 (6.8%)	38 (9.6%)	32 (9.1%)	16 (6%)	16 (9.5%)	9 (10.5%)	3 (6.38%)	4 (10.2%)	4 (5.7%)	179
2014	17 (26.9%)	31 (15.4%)	45 (12.7%)	47 (11.9%)	35 (10%)	40 (15.2%)	25 (14.9%)	12 (14.1%)	8 (17%)	4 (10.2%)	15 (21.4%)	279
2015	9 (14.2%)	18 (8.9%)	58 (16.4%)	46 (11.7%)	39 (11.1%)	32 (12.1%)	17 (10.1%)	5 (5.8%)	4 (8.5%)	9 (23%)	14 (20%)	251
2016	5 (7.9%)	16 (7.9%)	43 (12.2%)	45 (11.4%)	38 (10.8%)	38 (14.4%)	21 (12.5%)	11 (12.9%)	5 (10.6%)	3 (7.6%)	11 (15.7%)	236
2017	8 (12.6%)	33 (16.4%)	39 (11%)	39 (9.9%)	35 (10%)	39 (14.8%)	27 (16.1%)	15 (17.6%)	13 (27.6%)	6 (15.3%)	8 (11.4%)	262
2018	4 (6.3%)	20 (9.9%)	27 (7.6%)	36 (9.1%)	37 (10.5%)	28 (10.6%)	27 (16.1%)	12 (14.1%)	5 (10.6%)	8 (20.5%)	9 (12.8%)	213
Total	63 (3.10%)	201 (9.90%)	352 (17.33%)	393 (19.35%)	350 (17.24%)	263 (12.95%)	167 (8.22%)	85 (4.18%)	47 (2.31%)	39 (1.92%)	70 (3.44%)	2030 (100%)

Authorship Pattern of Publication

Table 5 depicts the authorship pattern for the period 2009-2018. The analysis of the table shows that the contribution is 3.10%, two author share is 9.90%, three author share is 17.33%, four author share is 19.35% , five author produces is 17.24%, six author share is 12.95%, seven author is 8.22%, eight author contribution 4.18, nine author share is 2.31, ten author contribution 1.92%, More than ten author 3.44% of the total articles 2030 it shows that multiple authored research articles have made major contribution in the field of crystallography in India.

Pattern of Co-Authorship Indexes CAI

Table 6: Pattern of Co-Authorship Indexes CAI

Year	Single	CAI	Two	CAI	Multi Authors (3&4)	CAI	Mega (>4)	CAI	Total	CC
2009	6	156	9	56	66	107	70	99	151	0.7
2010	5	7	11	77	67	122	52	83	135	0.68
2011	0	0	20	129	55	92	72	105	147	0.08
2012	3	66	16	85	70	97	88	107	177	0.72
2013	6	132	27	143	62	85	84	101	179	0.7
Total	20		83		320		366		789	
2014	17	120	31	116	92	94	139	94	279	0.68
2015	9	70	18	75	104	118	120	90	251	0.67
2016	5	41	16	71	88	106	127	101	236	0.7
2017	8	60	33	132	78	84	143	103	262	0.7
2018	4	36	20	98	63	84	126	112	213	0.31
Total	63	–	118	–	435	–	655	–	1241	–

The Collaborative Index, and collaboration coefficient were calculated based on year wise input of data.

Collaborative Index (CI)

Calculation:

$$CC = \frac{(f1)1+ (f2)2+(f3)3+\ldots+(fk)k}{N},$$

where f1, f2, f3, . . . = number of authors, N = Number of publications in that year.

Table 6 shows the distribution of output by Single, Multi and mega authored papers besides the values of the co-authorship index (CAI) and collaboration coefficient (CC) for the entire data was divided into 2 blocks 2009-2013 and 2014-2019. The average value of CC for crystallography is 0.68. However, the value of CC is showing increasing and decreasing trends in the two block years.

Distribution of Most Prolific Authors

The authors having 10 or more publications during 2009-2018 are shown in table 7, along with their number of publications, citations, CPP and h-index. Butcher Rj So, is the most productive author with 65 publications, 870 citations and 13.38 citation per publication followed by Drew Mgb with 63 publications, 870 citations

Table 7: Distribution of Most Prolific Authors

Sl.No.	Author	Total No. of Publication	Total No. of Citations	CPP	H-Index
1	Butcher Rj	65	870	13.38	19
2	Drew Mgb	63	870	13.80	19
3	Kumar A	55	430	7.81	11
4	Kumar S	55	570	10.36	14
5	Singh A	48	431	8.97	11
6	Singh N	48	630	13.12	17
7	Sharma Rp	47	380	8.08	10
8	Venugopalan P	43	327	7.60	10
9	LobanaTs	36	706	19.61	11
10	ChakravartyAr	33	1038	31.30	19

and 13.80 citation per publication, Kumar A with 55 publications, 430 citations and 7.81 citation per publication, Kumar S with 55 publications, 570 citations and 10.36 citation per publication, Singh A with 48 publications, 431 citations and 8.97 citation per publication.

High Productivity Research Areas

Table 8: High Productivity Research Areas

Sl. No.	Research areas	Total No. of Publication	% TP	H-Index	Total No. of Citation	Average Citations per
1	Chemistry	1,494	73.59 %	52	21,072	13.17
2	Crystallography	286	14.08 %	30	3937	12.46
3	Biochemistry Molecular Biology	256	12.61 %	29	3410	12.63
4	Materials Science	139	6.84 %	21	1589	11.03
5	Pharmacology Pharmacy	106	5.22%	17	1265	11.29
6	Biophysics	103	5.07 %	25	2143	19.48
7	Physics	83	4.08 %	15	931	10.58

Above Table 8 shows high productivity subjects which are contributing more than 80articles. Among subjects, the highly productive subjects were chemistry with 1,494 Publications and 21072 citations 13.17 citations per publication, Crystallography with 286 Publications and 3937 citations 12.46 citations per publication, Biochemistry Molecular Biology with 256 Publications and 3410 citations 12.63 citations per publication.

Language wise Distribution of publications

Table 9: Language Wise Distribution

Sl. No.	Language	Total No. of Publication	% TP	H-Index	Total No. of Citation	Average Citations
1	English	2,030	100.00	58	27,930	12.93

Above table 9 shows that the entire Crystallography publications referred in this study were published in English language only with 2030 (100%) Publications, 27,930 citations.

6. Conclusion

Crystallography is one of the very important subjects for Research in the present international development. Especially the crystal structure analysis helps the mankind in drug design. Quite a lot of research is going on in this field in various laboratories of India. For any nation knowledge is power and it is our scientific knowledge that determines our power in the International level. Though it is commendable that India stands in sixth position as regards to Crystallography research we require further more contribution in this field to become a developed nation from the present tag of developing nation. With the interest shown by the Government for Higher Education and Research in the nation, we can look forward for more breakthroughs in scientific knowledge and inventions.

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WOMEN EMPLOYMENT STATUS IN ORGANIZED SECTOR: AN EMPRICAL STUDY WITH REFERENCE TO VELLORE DISTRICT, TAMIL NADU

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Abstract

This paper describe the women employment status in organized sectors in India particularly Vellore District, Tamil Nadu. Objective of the study is to identify the total member of women employed in organized sector in India and to know the women employment in organized sector by Industry division. Methodology of the study is in order to test the specific objective of investigation, data are collected from primary and secondary sources through a structured questionnaire. Therefore, this study is descriptive in nature and based on primary and secondary data. Findings there are many openings and opportunities emerged in various organized and un-organized sectors due to globalization. Lack of proper education is the hindering factor. Indian women have to be given modern education and professional skills. The experiences of professional women in most of the developing countries indicate that the problems faced by them are essentially the same. Suggestions were given that the Nation develops if the womens are developed. So it is the first and foremost duty of our Government to pay attention for the well-being of the women community. A number of measures have been adopted by the Government for their welfare. But in some cases, womens interest is not protected.

Keywords: Organizing Sectors, Women Workers, Employment Industry Division.

1. Introduction

During this 21st century women's involvement for employment is vast compared with previous two decades. Mahatma Gandhi National Rural Employment Guarantee Act (MGNREGA): MGNREGA has played a remarkable role in employment of women

workers in organized sector. It has created better working conditions same wage to women and men. All India Democratic women's Association conducted a survey in 1989 in Pune city which reveals that women are involved in different types of home-based work as much as 150 occupations. It includes works like making flower garlands, folding paper for the printing industry, supplying chapattis to caterers, making agarbattis, weaving plastic seats for chairs, deseeding tamarind and packaging sweetis etc., Formal and informal surveys reveal that the workers in unorganized sector normally earn in the range of Rs.80 to 100 per day. Few of them would earn more in seasonal employments but the total earning would be around the same. To meet their needs, they are forced to work longer and harder. This scenario exists particularly, with the self-employed jobs like vendors, rag pickers and petty traders. They start their work in the early hours of morning to late in the night irrespective of the difficult working conditions. During 1970s, it had become quite obvious that some of the laudable objectives embodied within the constitution of general uplift of working conditions and equality for men and women, were being met only partially. There appeared to be an unmistakable long term trend of decline in women employments in modern organized industry were falling. This state continued up to 1980. In mid 1980s and 1990s, as the number of urban educated women aspiring for job increased, and as the strength of marriage as a universal and ubiquitous institution within India continued unbated, there was a rise in the number of working couples in urban settings.

2. Review of Literature

Saradamoni (1995) reports that female laborers' mostly from Kerala in the fish processing industries and in Gujarat are subject to various forms of hardship and exploitation at the hands of their superiors. **Saradamoni, K (1995)** opines women in our society have so for had only a secondary status and the economic dependence of women upon men is one of the primary reasons which has pushed them into the background and resulted into their secondary status both within and outside the family. **Sundaram (2000)** explains in India, the formal sector which received significantly large resources has failed to provide employment to the growing labour force, resulting in the problem of labour force explosion. Under these circumstances the surplus labour force has been forced to generate its own means of income and employment. This new class of petty-boiurgeosis ie engaged in a variety of economic activities. **Padma(2002)** indicates women workers in domestic services in 1999-2000 constituted 3.2per cent of the workforce and this comprised 39,25,000 workers. With this there has been a need for domestic servants to help the professionals in their daily chores.

3. Objectives

The following of the main objectives for the study.

- To know the status of the women participation in employment
- To indentify the Number of women employed in industry division wise
- To understand the effects of globalization on developments in the women workforce in India over the years
- To inspect the growth rate of women in organized sectors
- To analyses the growth rate of women in organized sectors industry division wise
- To assess the socio-economic conditions of the women workers in organized sector in the study areas.

4. Scope of the Study

The area coverage of this study was three taluks were selected Viz, Vellore, Gudiyatham and Vaniyambadi and each taluk two village Panchayats were selected. In Vellore taluk, Karugampathur and Thellur are selected, in Gudiyattam taluk, two village panchayats, Kondasamudram and Seevur, are selected. In Vaniyambadi taluk, Alangayam Panchayat, two village Panchayats viz, Vallaambattu and Vellakuttai wre selected in the Vellore District of Tamil Nadu, with specific focus on women laborers in the unorganized sector viz. as leather industry, service and agricultural sectors. The study emphasized different socio-economic condition, working conditions and problem faced by women laborers in the unorganized sector of Vellore District of Tamil Nadu was the centre of the study.

5. Research Methodology

In order to test the specific objective of investigation, data were collected from primary and secondary sources through a structured questionnaire. Therefore, this study is descriptive in nature and based on secondary data and primary data. In the first stage, In this study exploratory approach has been adopted and data are collected from secondary sources. In the second stage primary data relating to socio economic condition, working conditions, problem faced by women laborers and other related data collected from sample women laborers in the unorganized sector through a well-structured questionnaire.

6. Analysis of Data & Discussions

6.1. Work Force Participation Literacy and Population Growth

As per census 2011, India's working population constitute 32 per cent of the working population. Majority of working women are crowded in the unorganized sector. As

per report, presented at the 4th world conference on women in Beijing in 1995, only 4 per cent of all the working women are in the organized sector. This means that only about 0.005 per cent of India's population comprises of working women in the organized workforce.

A comparative statistical profile relating to women workforce participation in India is shown in table 6.1. This means that only about 0.005 per cent of India's population comprises of working women in the organized workforce table 7.1 revels that the total women at participation rate increased from 14.2 per cent in 1971 to 25.7 percent in 2001. The rate of rural women at work and urban women at work rate are also showing an increasing trend over the years. Among the total women workers, rural women participation at work is more compared with urban women. The workforce participation of women in urban areas is a mere 14 per cent as compared to 54 per cent for men. In rural areas, it is 31 per cent for women, where as it is 55 per cent for men.

Several factors are affecting either positively or negatively on work participation rate of women. Patriarchal tradition, influence of family, religious conservatism, economic condition, education, caste, status, etc are some factors which effects on women work participation rate. Another impediment of women labour participation is the immobility of labour.

Table 1: Work Force Participation Rates

Work Force Participation Rates		**1971**	**1981**	**1991**	**2001**	**2011**
Total	Persons	34.2	36.7	37.7	39.3	–
	Male	52.8	52.6	51.6	51.9	–
	Female	14.2	19.7	22.7	25.7	–
Rural	Persons	35.3	38.8	40.2	42	–
	Male	53.8	53.8	52.5	52.4	55
	Female	25.9	23.1	27.2	31	31
Urban	Persons	29.6	30	30.4	32.2	–
	Male	48.9	49.1	49	50.9	54
	Female	7.2	8.3	9.7	11.6	14

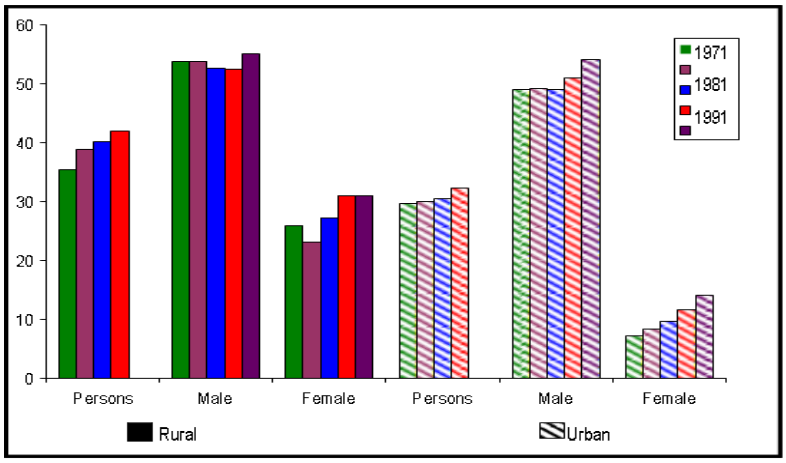

Figure 1: Work Force Participation Rates

Table 2: Sex Wise Growth of Population

Population (Millions)	1951	1961	1971	1981	1991	2001	2011
Total	361.09	439.23	548.16	683.33	846.3	1027.02	1210.19
Male	185.55	226.29	284.02	353.32	439.18	531.28	623.72
Female	175.53	212.94	264.14	330	407.12	495.74	586.49
Sex-Ratio	946	941	930	934	927	933	940

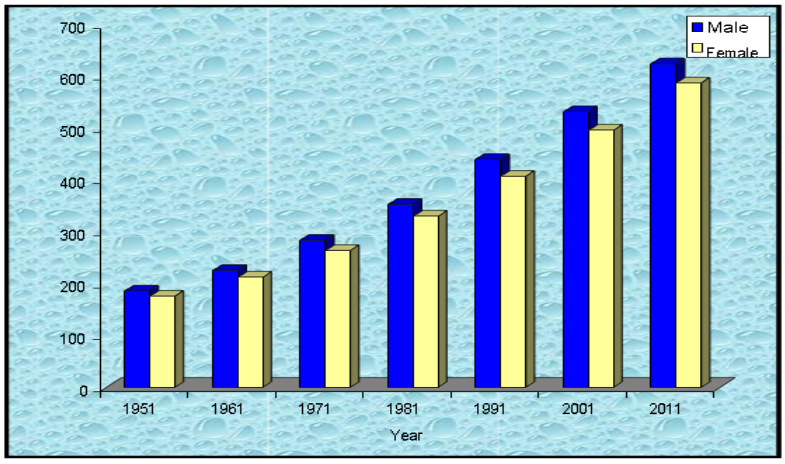

Figure 2: Sex Wise Growth of Population

Table 7.2 shows the sex wise growth of population, sex ratio and Table 7.3 shows literacy rates. The total population of the country has been increased substantially from 361.09 million in 1951 to 1210.19 million in 2011 census. The 21.54 per cent in 1991-2001 to 17.64 per cent in 2001-2011 census decades. Table also reveals that the women population has substantially increased over the years, whereas, female growth rate and the sex ratios are showing a declining trend. The overall literacy rate has increased from about 18.3 per cent in 1951 to about 74.4 per cent in 2011. Women literacy rate has also increased considerably over the years. The female literacy rate has showing an increasing trend of 8.9 per cent in 1951 to 65.46 per cent in 2011. Even through the literacy rate has increased over the years, the male female gap has not narrowed.

Table 3: Literacy Rates of Population

Literacy (%)	1951	1961	1971	1981	1991	2001	2011
Total	18.3	28.3	34.5	43.6	52.2	65.4	74.04
Male	27.2	40.4	46.0	56.4	64.1	75.9	82.14
Female	8.9	15.4	22	29.8	39.3	54.2	65.46

Source: Computed

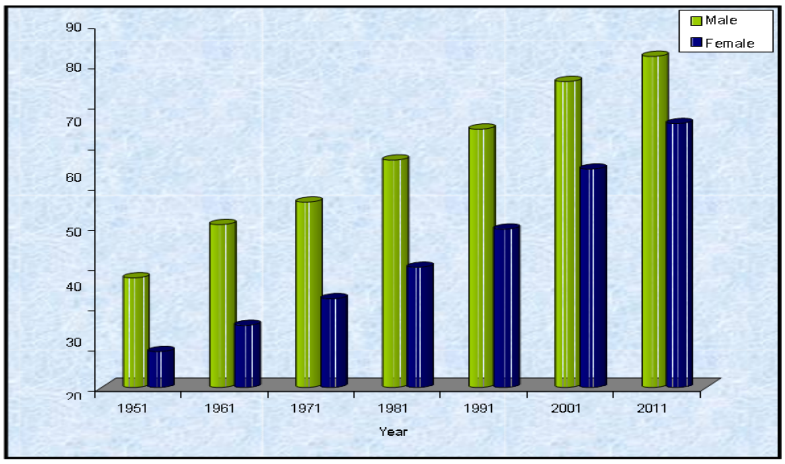

Figure 3: Literacy Rates of Population

The percentage of women employment in the organized sector is considerably less than the un-organized sector. Lack of education is one of the hindering factors to gain productive and remunerative employment. There is a huge education gap between organized and un-organized women workers. The agricultural workers have the lowest level of education. In un-organized sector, they work in various capacity- attached, bonded, casual, contract labour, workers in sweated industries like construction work, hand and power looms, beedi and cigar making, stone cutting, dhal and rice milling, pottery, crafts, match working, wooden work etc. The women employment in the Organized Sector in India is depicted in table 7.4

Table 7.4 indicates that out of the total number of women employed in organized sector in India, women employment in the public sector is more than the private sector. The women employment in the public sector has been increased from 26.00 lakhs in 1995 to 30.03 lakhs in 2006, and also increased substantially in private sector from 16.30 lakhs in 1995 to 21.18 lakhs in 2006. The increase in the employment in private sector may be due to the growth of Information Technology, Information Technology Enabled Services and BT industries. During this period these industries have adopted modern work styles, and family friendly measures, attracted women towards these industries.

Table 4: Women Employment in Organized Sector in India

Sectors		**1995**	**1996**	**1997**	**1998**	**1999**	**2000**	**2001**	**2006**
Public Sector	Total	194.7	194.3	195.6	194.2	194.2	193.1	191.4	–
	Male	168.7	167.9	168.3	166.6	166	164.6	162.8	–
	Female	26.0	26.4	27.3	27.6	28.1	28.6	28.6	30.03
Private Sector	Total	80.6	85.1	86.9	87.5	87	86.5	86.5	–
	Male	64.3	67.2	67.8	67.4	66.8	65.8	65.6	–
	Female	16.3	17.9	19.1	20.1	20.2	20.7	20.9	21.18
Total	Total	275.3	279.4	282.5	271.7	281.1	279.6	277.9	–
	Male	233	235.1	236.1	233.9	232.8	230.4	228.4	–
	Female	42.3	44.3	46.4	47.7	48.3	49.2	49.5	51.21

Source: Computed

Table 7.5 Shows that women employment in organized sector by industry division has shown an increasing trend in all the divisions of employment, women are employed the most in community; personal and social services, in the public sector, while they have the highest percentage of employment in the manufacturing sector followed by agriculture. Almost 400 million people (more than 85% of the working population in India) work in unorganized sector and of these about 120 million are women. According to an estimate, by the National Commission on Self-Employed Women (1988), of the total number of women workers in India, about 94 percent are in the informal or unorganized sector whereas just 6 percent are in the organized or formal sector. Thus there is no exaggeration in saying that the unorganized sector in India is the women's sector.

Table 5: Women Employment in Organised Sector by Industry Division (Thousands)

Industry Divisions	1981		1991		1996		2000	
	Total	Women	Total	Women	Total	Women	Total	Women
Agriculture, Forestry, Fishing and Hunting	1321	456 (34.5)	1447	498 (34.4)	1459	479(32.8)	1418	542(38.2)
Mining and Quarrying	948	87(9.2)	1099	79(7.2)	1100	81(7.4)	1005	65(6.5)
Manufacturing	6047	595 (9.8)	6333	597(9.4)	6787	876(12.9)	6616	1023(15.5)
Electricity Gas and Water	718	17 (2.4)	945	31(3.3)	988	38(3.8)	987	46(4.6)
Construction	1161	59(5.1)	1222	61(5.0)	1212	65(5.4)	1149	68(5.9)
wholesale and Retail Trade, Restaurants, Hotels	394	21 (5.2)	450	34(7.6)	479	41(8.5)	593	45(9.1)
Transport, Storage and Communication	2769	82(2.9)	3079	140(4.5)	3152	162(5.1)	3147	180(5.7)
Financial institution and Real Estate	944	80 (8.4)	1448	174(12.0)	1586	208(13.1)	1654	232(14.0)
Community, Personal and Social Services	8577	1397(16.3)	10712	2167(20.2)	11178	2476(22.2)	11494	2750(23.9)
Total	22879	2793 (12.2)	26735	3781(14.4)	27941	4426(15.8)	27963	4960(17.7)

Source: Computed

7. Findings

It is observed from the data analysis following major findings are expressed here

- It is indentified from the analysis that only about 0.005 per cent of India's population comprises of working women in the organized workforce.
- The analysis also reveals that the total women of participation rate increased from 14.2 per cent in 1971 to 25.7 percent in 2001.
- The rate of rural women at work and urban women at work rate are also showing an increasing trend over the years. Among the total women workers, rural women

participation at work is more compared with urban women.

- The workforce participation of women in urban areas is a mere 14 per cent as compared to 54 per cent for men. In rural areas, it is 31 per cent for women, where as it is 55 per cent for men.
- The analysis shows the sex wise growth of population, sex ratio and Table7.3 shows literacy rates. The total population of the country has been increased substantially from 361.09 million in 1951 to 1210.19 million in 2011 census.
- The figures of 2011 census reveals a decline in the rate of growth of population from 21.54 per cent in 1191-2001 to 17.64 per cent in 2001-2011 census decades.
- The overall literacy rate has increased from about 18.3 percent in 1951 to about 74.4 percent in 2011. Women literacy rate has also increased considerably over the years.
- The women employment in the public sector has been increased from 26.00 lakhs in 1995 to 30.03 lakhs in 2006 and also increased substantially in private sector from 16.30 lakhs in 1995 to 21.18 laksh in 2006.
- According to an estimate, by the National Commission on Self-Employed Women (1988), total number of women workers in India. About 94 percent are in the informal or unorganized sector whereas just 6 percent are in the organized or formal sector. Thus there is no exaggeration in saying that the unorganized sector in India is the women's sector.

8. Suggestions and Recommendations

It is observed that the overall literacy rate has increased and the workforce participation has raised over the years. Nation develops if the women's are developed. So it is the first and foremost duty of our Government to pay attention for the well-being of the women community. A number of measures have been adopted by the Government for their welfare. But in some cases, womens interest is not protected. Adult education programme for the women workers should be implemented for making them literate.

9. Conclusion

In this 21st century women's life style and cycle has changed due to their personal needs and social development. They have dual responsibility at their home and working place. Due to financial crisis and technology development, infrastructure needs, personal needs they have to contribute their life for work and residential needs. According to the study industry wise their contribution in creased from the year 1981 to 2000. It shows that

their responsibility and need is increased and they don't want to depend their spouse and parents. It means parents or spouse burden in the family may be reduced due to their contribution. The Government taking many initiatives and financial allocations for women's development. But it will not reaching them due to unawareness. To create awareness among the rural and semi urban areas is need of the hour.

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EMPIRICAL STUDY ON CONSUMER BEHAVIOUR TOWARDS SELECTED BRAND OF CARS IN VANIYAMBADI TOWN

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Abstract

Consumer Buying Behavior refers to the buying behavior of the ultimate consumers of the products or services. Knowledge of the consumer behavior is very essential for designing any marketing strategy. Understanding and adapting to consumer motivation and behavior is not an option it has become a necessity for competitive survival. Whenever, the marketing decisions are made without a real research of the consumer's behavior, based only on some assumptions and some economic or marketing ideas used previously, and the result can sometimes be good enough. This paper is going to exhibit different consumer behaviour when they come to buy selected brand of Cars in Vaniyambadi Town.

Keywords: Consumer Behaviour, MUV, SUV and Utility Vehicle.

1. Introduction

Consumer Buying Behavior refers to the buying behavior of the ultimate consumers of the products or services. Knowledge of the consumer behavior is very essential for designing any marketing strategy. Understanding and adapting to consumer motivation and behavior is not an option it has become a necessity for competitive survival. Whenever, the marketing decisions are made without a real research of the consumer's behavior, based only on some assumptions and some economic or marketing ideas used previously, and the result can sometimes be good enough.

The problem becomes important when old marketing practices don't function anymore and, there is a delay until marketers adapt to the new market situation. The current economic slowdown has stopped the previous consumption habits and now the market has to redefine where it's heading to and determine the emerging tendencies that will be profitable in the future.

2. Objectives of Research Article

1. To review the theoretical background relating in consumer behaviour in general and its relevance to behaviour of premium passenger cars, in specific.

2. To identify, study and analyses the variables that influence the behaviour of the consumers using premium passenger cars.

3. Statement of Problem

Understanding the consumer behaviour is a complex phenomenon as it involves variety of parameters and indicators that are to be reckoned with. The assessment of consumer behaviour pertaining premium car involves much more difficulties because of the involvement of esteem factors. Besides, the behaviour of human belong is always relating to reading the inner mind-set, one cannot easily intrude into it. Since it is invisible, cannot the gauged with a common yardstick. This study examines how the above things are relevant in the study of consumer behaviour across the sample respondents who have participated in this research.

Consumer Behavior is the study of how individuals, groups and organizations select, buy, use and dispose of goods, services, Ideas or experiences to satisfy their needs and wants. Marketer must understand both the theory and reality of Consumer Behavior. To further specify the definition of customer's attitude towards premium passenger cars, a set of attitude variables which potential buyers of luxury cars might hold was developed in discussion with premium car dealers.

4. Need and Importance of the Study

All the multinational car companies and considerable amount of the public revenue. Therefore, growth, development and survival of this industry is vital. The multinational car companies have well established production and logistic infrastructure so as to augment automobile demand of the Indian population, with their technology driven products and service edge. They frequently introduce more number of models which leads changes in the attitude and behaviour of consumers. This trend has created a volatile situation and high competitive environment among the indigenous and multinational car manufactures India. The marketers are struggling hard to market the premium products as the establishment of production facilities, distributions networks and other related activities involve huge investment.

The success in the above activities hinges on enhanced consumer satisfaction in cost and time effective method. This study specially attempts to unravel the truth behind in the complex task of measuring the consumer behaviour of premium car segment.

5. Research Methodology

This study has adopted descriptive analytical and exploratory methodologies. The study is mainly based on primary data collected directly from the sample respondents who have participated in this research, across the various sample products under the study. These data sets are also supplemented by journals, research articles, texts and publications from available sources within and outside India, pertaining to the research problem, covering different aspects of the research problem so as to pursue the various objectives set for this study.

The size of the sample for the study is determined to be one hundred and twenty five selected at random from the unknown population size, using the premium passenger cars across select brands. This study has been conducted at Vaniyambadi Town. As a metropolitan city, it consists of different socio economic classifications, covering different gender groups, income groups, educational background, different economic status with diversified culture, using the premium cars. Besides, almost all the leading brands have their sales, distribution, and service facilities. The present researcher belongs to Vaniyambadi Town and pursuing the research in the institution located in the heart of Vaniyambadi Town, the choice of study area as Vaniyambadi Town can be reasonable justified.

6. Review of Literature

Dr. Govind P. Shinde, Dr. Manisha Dubey (Research Entitled: Automobile Industry and Performance of Key Players): This study represents the figures of Indian automobile industry during the period 2005 to 2010. The study has been conducted considering the segments such as passenger vehicle, commercial vehicle, utility vehicles, multi-purpose vehicles, two wheelers and three wheelers. All the sections concisely explain the current and future market trends, the developments in the Indian automobile market. The methodology used to find the trends and the market share of the Indian automobile industry. The researcher for the said purpose, take into account, the past and current trends in an economy, and more specifically in an industry, to bring out an objective market analysis.

Satish K. Batra, S. H. H. Kazmi (Book Entitled: Consumer Behaviour (text and cases): The author in this book presents an in-depth study of consumer behaviour through several case studies. It is revealed that, consumer behaviour is an applied science. Though, the nature of the subject is such that, there are few definitive answers. Also, the study of consumer behaviour goes well beyond the mere act of acquiring or using the product or service. The study includes of how having or not having things affect our lives and how our possession or use of products or services influences the way we feel about others and ourselves.

7. Data Analysis and Results Discussion

Table 1: Friedman Test for Significant Difference among Mean Ranks towards Consumer Performance of Car users

Consumer performance of car users	Mean Rank	Chi-Square value	P value
Cost	4.94		
Fuel Consumption	3.35		
Brand	3.85		
Comfort	3.34	**88.607**	$< 0.001^{**}$
Utility	3.98		
Durability	3.93		
Quality	4.60		

Note: ** Denotes significant at 1% level

Interpretation

The above said table has factors of consumer performance of car users in Vaniyambadi Town. There are seven factors into this variable namely cost, fuel consumption, brand, comfort, utility, durability and quality. The mean rank to all these items are 4.94, 3.35, .85, 3.34, 3.98, 3.93 and 4.60. The highest mean rank is given to quality. Therefore, quality of car matters as far as performance of consumer who uses cars. While chi-square value witnessed here is 88.607 and it is significant at 1% level of significance and null hypothesis is accepted due to values of chi-square.

Table 2: Friedman test for significant difference among mean ranks towards Consumer Satisfaction of Car user

Consumer Satisfaction of car user	Mean Rank	Chi-Square value	P value
Service Facility	2.46		
Resale Value	2.37		
Availability	3.29	105.890	$< 0.001^{**}$
Performance	3.89		
Availability of Funds	2.99		

Note: ** Denotes significant at 1% level

Interpretation

The above table which was prepared in view of data collected through questionnaire. Analysis was made in such a way that response of various factors under the variable

of consumer satisfaction of car users. They are indicated by service facility, resale value, availability, performance and availability of funds. From the mean score, the first rank is given to performance, second rank is given to availability, and third rank goes to availability of funds and other two factors yield least mean score as they are not gaining momentum through analysis. Besides, null hypothesis is accepted as there is no significant relationship between the factors of consumer's satisfaction of car users.

8. Findings

There are seven factors into consumer preference namely cost, fuel consumption, brand, comfort, utility, durability and quality. The mean rank to all these items are 4.94, 3.35, .85, 3.34, 3.98, 3.93 and 4.60. The highest mean rank is given to quality. Therefore, quality of car matters as far as performance of consumer who uses cars. While chi-square value witnessed here is 88.607 and it is significant at 1% level of significance and null hypothesis is accepted due to values of chi-square.

Analysis was made in such a way that response of various factors under the variable of consumer satisfaction of car users. They are indicated by service facility, resale value, availability, performance and availability of funds. From the mean score, the first rank is given to performance, second rank is given to availability, and third rank goes to availability of funds and other two factors yield least mean score as they are not gaining momentum through analysis. Besides, null hypothesis is accepted as there is no significant relationship between the factors of consumer's satisfaction of car users.

9. Suggestions

The change in consumer preference was mainly due to fuel efficiency, as also design and technological improvement. Though, the newer versions of MUV's cars are slowly reviving the market for small car, the market share may not reach to the previous mark for many car manufacturers. Therefore, it is suggested that they must practice to have a constant urge to upgrade and keep pace with the changing times, as this would give organization the competitive advantages or cutting edge over the competition.

Consumer preferences have changed the demand pattern in other vehicle segments too, driven mainly by design and technology. Indian auto majors need to address the changing consumer preferences and suitably modify the design or technological improvement to augment their market share. Similarly, the service centre must be ready with all type of spare parts all over the time. After sale service has to be improved and service centers to be started even in rural areas so as to face the competition existing in the MUVs segments. Car manufactures of Mahindra MUV's and Toyota Innova must realize the fact that there is a heavy demand for these cars in the market. The supply has to be improved to meet the demand of the customers. Similarly they must

try to maintain reasonable price of the MUV's, as this is the key factor in customer buying decision. From the analysis it has observed that there is very less advertising for MUV's / SUV's segment cars in India. The advertising has to be done repeatedly so that the brand awareness could be maintained and new customers are attracted. This helps in improving the market share. Marketers can also introduce low installments and low down payment schemes to attract more people to buy MUV's / SUV's segment cars.

10. Conclusion

In the current study it has understood that the MUVs / SUVs 'Segment Cars' have attracted a large users with the ruggedness and multi utility features of the car, it has attracted the customers who were having large family size, business class and sports customers. From the detailed study it could be revealed that the MUVs section is the one that invites the maximum number of luxury features and other similar unique features of safety and much more.

The Sedan segment in the Indian market started to mature recently with the sudden growth in the economy in the Indian families. As the buying capacity increased so did the other major car making companies started to introduce their best sedans in their stable for the Indian market. The MUV / SUV models of different manufacturer are being launched in the Indian market they are even getting quick makeovers so that they are the four runners in the race to grab the biggest share in the pie of Indian car market.

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CUSTOMER SATISFACTION TOWARDS ONLINE SHOPPING OF ELECTRONIC GOODS (A STUDY WITH REFERENCE TO TIRUPATTUR DISTRICT)

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Abstract

Customer satisfaction, a business term, is a measure of how products and services supplied by a company meet or surpass customer expectation. It is seen as a key performance indicator within business and is part of the four perspectives of a balanced scorecard. In a competitive marketplace where business competes for customers, customer satisfaction is seen as a key differentiator and increasingly has become a key element of business strategy. There is a substantial body of empirical literature that establishes the benefits of customer satisfaction for firms. Customer satisfaction refers to the extent to which customers are happy with the products and services provided by a business. Customer satisfaction levels can be measured using survey techniques and questionnaires. Gaining high level of customer satisfaction is very important to a business because satisfied customers are most likely to be loyal and to make repeat orders and to use a wide range of services offered by a business. This article throws light on customer satisfaction towards online shopping of electronic goods at Tirupattur District.

Keywords: Customer Satisfaction, Prompt Delivery, Amazon and Flipkart.

1. Introduction

Customer satisfaction, a business term, is a measure of how products and services supplied by a company meet or surpass customer expectation. It is seen as a key performance indicator within business and is part of the four perspectives of a balanced scorecard. In a competitive marketplace where business competes for customers, customer satisfaction is seen as a key differentiator and increasingly has become a key element of business strategy. There is a substantial body of empirical literature that establishes the benefits of customer satisfaction for firms. Customer satisfaction refers

to the extent to which customers are happy with the products and services provided by a business. Customer satisfaction levels can be measured using survey techniques and questionnaires. Gaining high level of customer satisfaction is very important to a business because satisfied customers are most likely to be loyal and to make repeat orders and to use a wide range of services offered by a business.

Customer satisfaction means giving the customers what they really want, when they want it and the way they want it. It involves understanding customer expectations and meeting them fully. it can be defined as an outcome of purchase and use resulting from the buyers comparison of rewards and the cost of the purchase in relation to the anticipated consequences.

Customer is an individual or an organization. Their requirements are very similar.

- Conformance of services to their requirements and its performance in actual stage.
- Competitive prices.
- Quality and reliability.
- Prompt delivery.
- Service.

2. Statement of Problem

The researcher has to find the level of satisfaction of the customers at the time of usage of major electronic goods such as Laptop, Personal Computer, Notepad, Mobile Phones and Television. Satisfaction is the prime factor that increases the volume of the sales of the company. There are many issues in relation to customer satisfaction which arise from the time purchase of electronic goods is made till the usage of such goods. One of the main issues pertaining to customer satisfaction is expectation. However, sometimes customers cannot get access to the concerned websites due to lockage of pop up and disruption of connectivity.

Customers go through various websites and execute the purchase after choosing the specific online platform but such online platform cannot give proper assurances due to lack of face to face interaction. So, this study is very specific on highlighting customer satisfaction towards online shopping of selected electronic goods in Tiruppatur Town.

3. Objectives of the Study

- To study the reasons for consumer preferences of online shopping of selected electronic goods in Tirupattur Town.
- To study the motivational factors in trade to buy the electronic goods via online.

4. Need for the Study

In today's competitive market, the company has to focus on customer satisfaction. Only then, he is able to capture the market and promote the sales across the entire region in the country. With regard to knowing the customers mentality, the company has to study the market and sometimes the researcher may assist in providing the details pertaining to this to the company which may be considered as valuable information. So any company who has to increase the satisfaction of the customer has to make academician to undergo the research in his own premises. The study becomes more important in giving due rise to the satisfaction of the customer. Customers want to be treated right. Plenty of research proves that the majority of customers will choose the company that made them satisfied even if it offers higher prices over a cheap but low quality service option.

So take the effort to satisfy customers with excellent service, as it is even more important than offering lucrative prices. Moreover, increases in costs are easier to justify when clients are satisfied at every stage of the interaction.

5. Scope of the Study

There are plenty of opportunities available by way of studying the customer satisfaction. This is a situation at which the company might know the position of the customers in buying their product. Besides, the company can handle the situation independently to solve the problems amicably. Even the company in future may hold the meetings, conference, discussion etc. in boosting up the customer satisfaction. Study about customer satisfaction is important for business enterprises due to its long survival in the industry. Unless customers get satisfied, survival of our business is no longer and will get short lived.

Online shopping is a platform where customers rapidly start buying electronic components because of being many lucrative offers as compared to offline shopping. Now a days, even layman too prefer to buy goods through online over offline. This is because of price variations, various easy mode of payment options, quality and prompt delivery of goods.

6. Research Methodology

The researcher in all, selected the sample size of 80 customers who are the frequent online buyers of electronic and other goods in and around Tirupattur town. The database of the customers was collected through major webportal like Amazon, Fliptkar and Snapdeal through these portal customers had frequent online shopping. Well-structured questionnaire using google forms were developed and circulated among the target sample and totally 120 questionnaires were sent to the mail id of the respondents who

usually buy their electronic goods via online platform and only 80 filled in questionnaire were received back and used for data analysis. The researcher goes through various books on topic oriented, articles published by various authors, different websites needed for his study which are all mentioned in bibliography.

The research design is the frame work for the rest of process. The research design used for this study is the elaborative and data analysis research design, because this research not only describes something such as demographic characteristics of consumers who are using online electronic goods. Further the research is designed to employed percentages, weighted average method and simple statistical methods.

The sampling method adopted in this study is convenience sampling. Since it is left to the freedom of the customers who are the frequent online buyers of electronic goods in and around Tirupattur Town. The researcher would like to put forth this method rather than any other methods. Sample Unit is a place where research study is conducted. Since research work is carried out across Tirupattur Town. Sample Unit is Tirupattur where 80 customers are randomly selected and data collected. Researcher has totally selected 80 customers from Tirupattur Town who are constant online buyers of electronic goods via various online platforms such as Amazon, Flipkart and Snapdeal.

7. Review of Literature

The reason an organization is interested in the satisfaction of its customers is because customers purchase the organizations products. Te organization is interested in retaining its existing customers and increasing the number of its customers. Customer satisfaction is an ambiguous and abstract concept and the actual manifestation of the state of satisfaction will vary from person to person. The state of satisfaction depends on a number of both psychological and physical variables **Kellet and Godwin (2007)**.

The level of satisfaction can also vary depending on other options the customer may have and other products against which the customer can compare the organization's products **Metha (2004)**.

8. Analysis and Results Discussion

Table 1: Kaiser-Meyer Olkin for Customer Satisfaction of the Purchase of Electronic Goods in Tirupattur District

Kaiser-Meyer-Olkin Measure of Sampling Adequacy		.724
Bartlett's Test of Sphericity	Approx. Chi-Square	215.573
	Df	48
	Sig.	.000

Interpretation

The Kaiser-Meyer-Olkin Measure of Sampling Adequacy is a statistics that indicates the proportion of variance in variable that might be caused by underlying factors. High values (close to 1.0) generally indicate that a factor analysis may be useful with data. If the value is less than 0.50, the result of the factor analysis probably won't be very useful. In this study, the value of Kaiser-Meyer-Olkin Measure of Sampling Adequacy is 0.724 (72.4%) which is adequate.

Bartlett's tests the hypothesis that correlation matrix is an identity matrix, which would indicate that variables are unrelated and therefore unsuitable for structure detection. A small value (less than 0.05) of the significance level indicates that a factor analysis may be useful with data.

Table 2: Total Variance Explained for the Customer Satisfaction towards Online Shopping of Electronic Goods

Component	Initial Eigenvalues			Rotation Sums of Squared Loadings		
	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %
1	2.749	30.541	30.541	2.135	23.727	23.727
2	1.292	14.359	44.900	1.821	20.234	43.961
3	1.139	12.654	57.554	1.223	13.593	57.554
4	.903	10.029	67.584			
5	.737	8.192	75.776			
6	.685	7.617	83.392			
7	.545	6.051	89.444			
8	.493	5.473	94.917			
9	.457	5.083	100.000			

Factor analysis extracts maximum common variance from all variables and puts them into a common score. In the Total Variance Explained table we see that 3 factors have been extracted that have Eigen value greater than 1. Eigen values explain the variances of the factors and values greater than one represent considerable variance, forming significant factors. The above table shows that the total variance explained is 57.554%. This is appropriate for factors analysis. The 57.554% variance was explained by the 3 extracted components.

9. Findings

The Kaiser-Meyer-Olkin Measure of Sampling Adequacy is a statistics that indicates the proportion of variance in variable that might be caused by underlying factors. High values (close to 1.0) generally indicate that a factor analysis may be useful with data.

If the value is less than 0.50, the result of the factor analysis probably won't be very useful. In this study, the value of Kaiser-Meyer-Olkin Measure of Sampling Adequacy is 0.724 (72.4%) which is adequate.

Brand Image is taken in to account while purchase is executed. Among the total variables, nine variables are identified that increase the satisfaction to a certain extent at the time of online purchase of electronic goods. The most dominating factor that increases the satisfaction of customer is online shopping is convenient and easy to use whose factor score is .892 while the next immediate element is Brand Image is taken in to account while the purchase is executed (.797).

10. Suggestions

Consumers should listen to the notification and get close to the dealers to know more about the product. Information like discount, features, and characteristics should be clearly explained to the customers before the purchase is made. So that customers will trust the manufacturers and they will have long time associations due to the ethical practices of online dealers. Sellers once sell their products should follow up the customers after the sale and extend the service either at free of cost or at some cost as and when required. They should offer the free services within warranty period and maintain the data base of the customers. When the next service falls due, that should be intimated to the concerned customers.

Prices of the electronic goods should be visible enough. But in some cases, prices of the electronic goods are not properly displayed and when the products are delivered, they are offered at the cost beyond the expectation of the customers. Proper banking network should be made and if necessary, credit facility should be arranged to the trustworthy customers. EMI facility also should always be made available. The same should be intimated to the customers.

11. Conclusion

As part of this study, researcher has made an attempt to bring out the customer satisfaction towards the online purchase of electronic goods in Tirupattur. Online purchase is really getting convenient now a days due to mode of its operation by the sizeable population. There are many options left with online purchasers. These are the reasons why people choose the online purchase. The primary benefit of online purchase is that it removes the involvement of middlemen who adds commission in the between the cycle of transaction. When the product is made available ultimately, they are offered at higher prices. But online purchase eliminates the role of middlemen and it makes the products available at fair prices.

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TEACHERS' INVOLVEMENT IN STUDENTS' MENTORING - A Study of University & College Teachers in India

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Abstract

This research article talks about relationship of mentors with mentees and suggests for better implementation of the concept and to realise more effectiveness in it. Primary data has been used for the purpose of study using a questionnaire. To be simpler and more logical for even layman, the researchers have restricted the analysis only to 'simple percentile'. The study is completed with the thirty samples drawn by convenience sampling technique. The results highlight on the lacuna and the probable measures for its improvement.

Keywords: Mentoring, Student Mentoring, Teachers' Involvement, Teacher as Mentor.

1. Introduction

Mentoring is a system of semi-structured guidance whereby one person shares his/her knowledge, skills and experience to assist others to progress in their own lives and careers. Mentors need to be readily accessible and prepared to offer help as the need arises - within agreed bounds. Educational institutions particularly Universities and Colleges are not an exception to this concept. In earlier days it was presumed that the concept of mentoring has nothing to do with educational institutions and constrained its scope only to organisations. Later, it was realised that the concept is aptly used in school kids particularly of youngers studying primary level schooling and later its significance was much realised in the elderly students of high and higher secondary level and slowly

the same was found important rather more important in the educational institutions of higher education be it a polytechnic, arts and science colleges, engineering colleges, medical colleges and even Universities of all kind. Now mentoring finds its place in almost every walk of life.

2. Need and Significance of the Study

Order of the day compelled every educational institution irrespective of the level at which it functions and the pupils for whom it meant, to have this concept of mentoring in their premises and colleges and universities are not an exception to it. The concept of mentoring in educational institutions gained momentum right from the beginning of twenty first century itself when many western countries realised the importance of it and introduced in their schools and colleges. In India the concept was introduced in technical institutions first and slowly extended to institutions offering non-technical courses. Educational institutions offering courses of arts and science nature be it a university or college throughout India also uses this concept of mentoring to gain educational benefits. Many institutions have this concept without taking it seriously and as a result of that fail to enjoy the full fruitfulness of the concept.

3. Research Problem

The regulations of courses country wide are evident that the concept of mentoring exists in the system. Quantitative data are verily available in the internet or respective websites of the institutions or the websites of official clusters in any form and databases of regulating authority like University Grants Commission and such other academic bodies. Qualitative data are comparatively less available which is very much equivalent to nil. When someone talks about qualitatively, it is a must for him or her to view the concept from psychological perspective in the sense the relationship perspective attached to the concept of mentoring. In this research work, a humble attempt has been made to study from this lagging perspective. The success or failure of the concept of mentoring is largely dependent on the relationship exist between the mentor and mentees. To be more specific the success or failure depends more on the commitment shown by the mentors towards the mentees. Hence, an urge realised to know the commitment of mentors in these institutions of higher education towards their respective mentees from a single aspect called relationship which is the base for other aspects of the concept. To get clear on this one should understand that mentorship requires involvement from both the parities to it the mentor and mentee. The mentorship is comparatively more successful when both the parties to mentorship are free to select the opponent. That is the mentors are allowed to select the mentees and mentees are also given sufficient freedom in selecting or rejecting the mentor while deciding

about. This scenario is much difficult rather impossible in the present Indian educational institutions because the respective governing regulations of the courses are designed in such a manner in most of the cases where a mentor is assigned without the mentees nod and are expected to be in the bond of mentor-mentee relationship either for the entire course period or at least for a defined period of time. In such a situation it becomes very much necessary on the part of the mentors to be more careful in exercising their powers while discharging their duties. It is their bounded responsibility to establish a good bond between himself or herself with the assigned mentee or mentees. This nature has raised a kind of problem that many mentors are just mentors for the name sake maintaining only official records by failing themselves in maintaining relationships. In this situation, if the mentors are not really committed enough towards their respective mentees, the purpose of mentorship will not surely be served. This problem has raised few research questions into the minds of researchers.

Do the mentors really attach to mentees?

Can the same be scaled?

Is it possible to increase the commitment by following some suitable suggestions? and if so, what are those?

4. Objectives of the Study

To get the answers for the above research questions, the researchers have framed the following research objectives.

1. To study the attachment of mentors with the mentees in the given setup.
2. To gauge the mentors' involvement in a very simple way.
3. To make suggestions to the mentors to increase their involvement.

5. Research Methodology

Research methodology has been presented in the following sub paragraphs.

5.1. Nature of Data

To fulfil the objective mentioned above the authors thought to get the help from both the primary data and secondary data. It would be very difficult to understand the research problem in a very clear way unless a brief understanding on the different concepts of mentoring is known and hence an attempt has been made to present the same using secondary data. For collecting the data on mentors' involvement, a specially designed questionnaire has been used.

5.2. Sample Size and Sample Methodology

The sample size has been fixed as thirty drawn from different corners of the Country. The convenience sampling technique has been adopted to enjoy maximum convenience on the part of the researchers. The researchers have contacted one Human Resource Development Centre of a north Indian University and obtained permission to collect the data from the participants of the then ongoing batches of Refresher Courses and Orientation Course. Through the course co-ordinators of Refresher Courses and Orientation Course, teacher participants who are mentors in their respective institutions and willing to participate in the research were enlisted and served the questionnaire. The HRDC though north based, were offering courses for teachers across India and therefore, the composition of samples constitute representation from all over India.

5.3. Questionnaire

Rubin's love and liking scale was used by Late Prof. V.M. Md. Anwer Basha, Former Vice-Principal & Head of the PG & Research Department of Commerce, Islamiah College (Autonomous), Vaniyambadi, Tirupattur District, Tamilnadu, India and designed a twelve statement questionnaire with modifications for a similar survey on mentoring in educational institutions of higher learning a psycho-analytical perspective in the year 2010. The same redesigned love scale has been used here for the purpose of study.

5.4. Validation of the Tool

For validating the tool used for the research study, reliability test named 'Cronbach Alpha Test' was carried out and the results showed a value of 0.892. Therefore, the tool used for the purpose of the study is very suitable to be used.

5.5. Statistical Tool Used

To make the study understandable not only to the learned people but also to layman, it has been decided not to use complicated statistical tools and to use only very simple and widely used simple tool of percentiles. The entire interpretations are based on the percentile-based frequency distribution.

5.6. Pilot Study

To test the feasibility of the usage of the said questionnaire, pilot study has been done with three teachers working in three different stages namely, tamilnadu, karnataka and kerala respectively. The responses obtained from these three teachers proved that the questionnaire does not require any change and therefore it has been decided to use the same research tool without any further modification in it.

6. Review of Literature

Margaret Andrews and Frances Chilton (2000) have done a study which is an account of a small pilot study conducted over a 3-month period which ascertained the views of staff nurses and students about the mentoring process. In particular, whether the possession of a teaching qualification influences the effectiveness of mentors. The research was conducted in a district general hospital in North Wales. The findings demonstrate that staff nurses with a teaching and assessing qualification consistently rate themselves as more effective and supportive than those without. Other findings show that students consistently rate their mentors positively irrespective of whether they held a teaching and assessing qualification and that students rate their mentors more positively than the mentors themselves. Although these findings are not generalizable in the accepted sense, they may be applicable to other practice settings. The findings and discussion indicate several implications for future practice including the need for more consistency in practice regarding the nature and purpose of mentorship, clear criteria and selection processes for potential mentors, including more extensive use of the Measuring Mentor Potential (MMP) scale as a predictive tool, a review of current mentor preparation programmes to align them with the needs of diploma and degree students and to ensure comparability of standards throughout the UK.

Pamela J. Kalbfleisch & Andrea B. Davies (1993) have involved in a study entitled 'an interpersonal model for participation in mentoring relationships'. This study develops and tests a conceptual model of the relationship between three interpersonal components and involvement in mentoring relationships. The model was found to be a good fit for forecasting protege involvement. For proteges, communication competence and selfesteem were both directly and indirectly related to participation in mentoring relationships. The indirect relationship was modified by perceptions of risk in intimacy. For mentors the best model manifested an indirect relationship between communication competence, selfesteem and participation in mentoring relationships. Perceptions of risk in intimacy moderated this indirect relationship. Implications for the study of mentoring relationships as interpersonal relationships are discussed.

Stacie Craft DeFreitas1 and Antonio Bravo Jr. (2012), have indulged in a research work titled The influence of involvement with faculty and mentoring on the self-efficacy and academic achievement of African American and Latino college students in which African American and Latino college students were surveyed to examine the influence of involvement with faculty and mentoring on self-efficacy and academic achievement. It was hypothesized that involvement with faculty and mentoring were related to greater academic achievement. It was suggested that the relationship of these factors was mediated by self-efficacy. Involvement with faculty and self-efficacy were significantly related to academic achievement. The relationship between involvement with faculty and better academic achievement was partially explained by higher self-efficacy. Possible explanations for mentoring not being predictive of

academic achievement in this sample were provided and the significance of faculty-student interactions was discussed.

Kathleen Duffy, Charles Dochety and et.al. (2000), have done a research work with the tile The Nurse Lecturers role in mentoring the mentors. This article reports on the results of a survey conducted early in 1999 investigating the effectiveness of current arrangements for mentor preparation and ongoing mentor support provided within adult placement areas within Greater Glasgow Health Board. A sample of 150 mentors was surveyed with a response rate of 47% (n=71). Results indicate that although mentors are generally satisfied with the current approach to mentorship preparation, the issue of support from both managers and academic staff is problematic. Respondents indicate that they wished to see lecturers visiting the practice placement areas and providing support, particularly in relation to assessment of students. Also highlighted in this study is the need for more effective communication between placement areas and academic staff.

7. Conceptual Definitions

7.1. Mentor

A mentor is a person or friend who guides a less experienced person by building trust and modelling positive behaviours. The word mentor comes from the character "Mentor" in Homer's epic tale, The Odyssey. Mentor was a trusted friend of Odysseus, the king of Ithaca. When Odysseus fought in the Trojan War, Mentor served as friend and counsel to Odysseus' son Telemachus. Riverside Webster's II New College Dictionary 1995 defines a mentor as "a wise and trusted teacher or counsellor". In this study the mentor refers to the in-charge teacher of college or university to whom a set of students (mentees) are assigned.

7.2. Mentee

Mentee is a person who is advised, trained, or counselled by a mentor. A mentee is someone who has identified a specific personal or professional goal and who believes that the guidance and help of a mentor and being held accountable to the mentor can help them achieve their goal. In this study mentee refers to the student pursuing higher education in university or college of arts and science stream who is assigned to a mentor teacher.

7.3. Mentoring

The dictionary meaning of the term mentoring is presented in the sentences. The act or process of helping and giving advice to a younger or less experienced person, especially in a job or at school. The activity of supporting and advising someone

with less experience to help them develop in their work. Employee training system under which a senior or more experienced individual (the mentor) is assigned to act as an advisor, counsellor, or guide to a junior or trainee. The mentor is responsible for providing support to, and feedback on, the individual in his or her charge. Mentoring is a system of semi-structured guidance whereby one person shares their knowledge, skills and experience to assist others to progress in their own lives and careers. Mentors need to be readily accessible and prepared to offer help as the need arises - within agreed bounds.

Mentors very often have their own mentors, and in turn their mentees might wish to 'put something back' and become mentors themselves it is a chain for 'passing on' good practice so that the benefits can be widely spread.

Mentoring can be a short-term arrangement until the original reason for the partnership is fulfilled (or ceases), or it can last many years.

Mentoring is more than 'giving advice', or passing on what your experience was in a particular area or situation. It is about motivating and empowering the other person to identify their own issues and goals, and helping them to find ways of resolving or reaching them - not by doing it for them, or expecting them to 'do it the way I did it', but by understanding and respecting different ways of working.

Mentoring is not counselling or therapy - though the mentor may help the mentee to access more specialised avenues of help if it becomes apparent that this would be the best way forward.

Mentoring in education involves pairing young people with an older peer or volunteer, who acts as a positive role model. In general, mentoring aims to build confidence, develop resilience and character, or raise aspirations, rather than to develop specific academic skills or knowledge.

Mentors typically build relationships with young people by meeting with them one to one for about an hour a week over a sustained period, either during school or college, at the end of the day, or at weekends. Activities vary between different mentoring programmes. While some mentoring programmes include some direct academic support with homework or other institutional tasks, approaches focused primarily on direct academic support are not covered in this strand.

7.4. Involvement

The dictionary meaning of the term 'involvement' is the fact or condition of being involved with or participating in something. The other meanings from different dictionaries are presented in the following sentences. Emotional or personal association with someone. The act of involving or the state of being involved. The act of sharing in the activities of a group. A connection of inclusion or containment. A sense of concern with and curiosity about someone or something.

Involvement or employee involvement can be defined as creating an environment in which an employee participates more in the day-to-day decision-making which leads to

a better relationship with the manager. More direct participation by employees helps the organisation to achieve its goals rapidly and effortlessly.

Employee involvement is not any quantitative tool or a goal of an organisation, it is more of a leadership tool or a thought which usually percolates from the top. This culture can only be adopted if senior managers are satisfied with more employees' participation in the day-to-day working of the company. For effective working, organisations should involve more and more people in some kind of decision-making or planning of activities. More involvement brings a sense of accomplishment in the minds of employees as well as increases their commitment level towards the organisation. The idea behind this concept is that employees who are already aligned with a set of work know what is best for the process or department they are working for. By engaging employees more, a firm shows that it values its employees; in turn it leads to a better commitment level from employees. Involving employees more would also lead to the dissemination of better ideas, which will result in higher productivity and better quality.

In this study involvement refers to the act of involving himself or herself by teachers of higher education in helping out and guiding the respective students as a component of mentoring activity.

8. Analysis and Interpretation of Data

The analysed data have been presented in the following table and the related interpretations follows.

Table 1: Frequency Distribution

S.No.			**SDA**	**MDA**	**N**	**MA**	**SA**
1	Attachment	Frequency	1	1	3	3	22
		Percentage	3.3	3.3	10	10	73
2	Level of Understading	Frequency	–	1	2	7	20
		Percentage	–	3.3	6.7	23.3	66.7
3	Expected Intelligence	Frequency	–	3	3	16	8
		Percentage	–	10	10	53.3	26.7
4	Communication	Frequency	1	1	–	5	23
		Percentage	3.3	3.3	–	16.7	76.7
5	Friendliness	Frequency	1	3	2	7	17
		Percentage	3.3	10	6.7	23.3	56.7
6	Satisfactory Relationship	Frequency	1	2	1	8	18
		Percentage	3.3	6.7	3.3	26.7	60

7	Reflection	Frequency	–	–	4	11	15
		Percentage	–	–	13.3	36.7	50
8	Stress Level (Attention Seeking / Attentiveness)	Frequency	6	4	4	8	8
		Percentage	20	13.3	13.3	26.7	26.7
9	Helping Tendency	Frequency	2	–	2	5	21
		Percentage	6.7	–	6.7	16.7	70
10	Relationship Happiness	Frequency	2	2	2	15	9
		Percentage	6.7	6.7	6.7	50	30
11	Anger Management	Frequency	2	2	3	10	13
		Percentage	6.7	6.7	10	33.3	43.3
12	Endurance	Frequency	2	2	3	13	10
		Percentage	6.7	6.7	10	43.3	33.3
SDA-Strongly Disagree, MDA-Moderately Disagree, N-Neutral, MA-Moderately Agree, SA-Strongly Agree							

8.1. Attachment

Attachment is a deep and enduring emotional bond that connects one person to another across time and space (Ainsworth, 1973; Bowlby, 1969). Attachment does not have to be reciprocal. Attachment theory explains how the parent-child relationship emerges and influences subsequent development. In this research context, emotional bond that connects teachers with their respective students across time and space is to be seen. In this teaching learning environment, reciprocal attachment from students is also expected.

73.3 per cent of the respondents have strongly agreed that Students and they are attached to each other'. A ten percent of the teachers have moderately agreed that they are attached to students. Totally, 83.3% have shown green signal for this attachment statement. Only 6.6 percent of the teachers have shown red signal for this statement that they are not attached to their respective students. Another 10 percent of the students have opted 'neutral' option in the scale which means that they have not tried so for to realise the attachment they have with their students. They are the people who discharge their duty of mentoring just as the task has been assigned to them. They are the people on whom a considerable work needs to be done to develop attachment.

8.2. Level of Understanding

The relationship between student and teacher plays a large role in the trajectory of a child's academic success and social development. Establishing a positive relationship

with their teacher helps a student feel more comfortable and safer in their classroom environments.

Understanding here refers to the mental wave length synchronisation between the teacher and the student in select situations particularly connected to teaching-learning process.

66.7% of the respondents have strongly agreed the statement 'there is understanding between me and my students'. Similarly, 23.3 per cent of the respondents moderately agreed the above statement. Therefore, totally, 90% of the respondents are having good understanding with their students. 6.7 % of the respondents have opted for Neutral option in the scale which means they are either not ready to understand the opponent or have taken seriously the requirement of understanding between teachers and the students. Only a meagre percentage (3.3) of the respondents have moderately disagree the said statement. These teachers require strong boost to inculcate the habit of developing understanding towards the students. It is very interesting to note that not even a single respondent has selected 'strongly disagree' category that means there is no single teacher who has not at all developed any understanding with the respective students.

8.3. Expected Intelligence

Intelligence has been defined in many ways: the capacity for logic, understanding, self-awareness, learning, emotional knowledge, reasoning, planning, creativity, critical thinking, and problem-solving. More generally, it can be described as the ability to perceive or infer information, and to retain it as knowledge to be applied towards adaptive behaviours within an environment or context.

Here, expected intelligence refers to the level of intelligence students are having. Of course, this is in tune with the expectations of the teachers. The above table shows that a total of 80% of the teachers agreed that the students are up to the expectations of the respective teachers in terms of intelligence. A 10% of the respondents have neutral selection that means either the teachers have not tried to test the students in terms of their intelligence or the students might be shy type that they might not have come forward to show their intelligence. Another 10% of the respondents have opted for 'Moderately Disagree' option and there is none who opted the option 'Strongly Disagree'.

8.4. Communication

Communication is simply the act of transferring information from one place, person or group to another. Every communication involves (at least) one sender, a message and a recipient. This may sound simple, but communication is actually a very complex subject. The transmission of the message from sender to recipient can be affected by a huge range of things. These include our emotions, the cultural situation, the medium used to communicate, and even our location. Here, communication refers to the information transmitted between the mentors and the mentees. The questions being

posed to the mentees, the questions raised by mentees, the answers for the above from the mentees and mentors, doubts being raised, the clarification of the above doubts, and all such conversations resulting in the fulfilment of the teaching-learning process come under the scope of this communication process.

It is interesting note that not even a single respondent opted for 'Neutral' category for the respective statement. That means the respondents are clear with respect to the statement 'I have no difficulty in communicating with my students'. A total of 93.4% of the respondents are agreeing to the said statement and only 6.6% of them are disagreeing to it. This clearly shows the good communication exist between the mentors and mentees.

8.5. Friendliness

Friendliness is a quality of openness and warmth that makes oneself feel welcome and at ease. The friendliness is evident from facial expressions, body language, and, most importantly, in the way one treats other people. Other words for friendliness include cordiality and kindness. It refers to the quality or state of being friendly. Here, friendliness refers to state of being friendly by teachers with their students.

Seventy percent of the teachers are agreeing to the statement 'I expect to always be friendly with my students' which means these teachers are really expressing friendliness when it comes to dealing with their respective students. 13.3% of the teachers are disagreeing to the above said statement which shows that these teachers are 'strict' kind of teachers who actually do not express their friendliness towards their respective students. Only a 6.7% of the teachers have opted for 'Neutral' option in the scale who are surely those teachers who do not like the concept of mentoring at all.

8.6. Satisfactory Relationship

The statement 'our relationship is most satisfying' simply refers to the satisfactory feeling of teachers towards their respective students in terms of accepting them as their mentees. They feel either happy or ok with their respective students. This statement talks about teacher-student relation - the academic relation between teachers and their students. Academic relation refers to a professional relation between instructors (teachers) and those they instruct (students).

Teacher-students' relationships should be based on trust, respect, and on the knowledge that it is a team effort. Students need to know they have to do their share of the work. If the teacher-student relationship is bad, the student won't do very well in the subject.

Eighty six point seven percent of the respondents are saying that they are satisfied with their respective students when it comes to teacher-student relationship. Only ten percent of the respondents are disagreeing to it. Proper motivation is required to such teachers. A meagre 3.3% of the respondents have opted for 'neutral' option in the scale.

8.7. Reflection

In teaching-learning environment, we reflect in order to learn something, or we learn as a result of reflecting, and the term 'reflective learning' emphasises the intention to learn from current or prior experience. Reflection is a type of thinking aimed at achieving better understanding and leading to new learning.

For the statement My main consideration is shaping my students how they would reflect, 50% of the respondents have strongly agreed while 36.7% of them have moderately agreed. Therefore, a total of 86.7% of the respondents have agreed that the mentoring process results in reflection. Students are getting better and better understanding which ultimately results in new learning. It is to note that apart from 13.3% of the respondents who are neutral for the statement, none have disagreed neither moderately nor strongly which means that every respondent except opted for neutral have no doubt about the reflective benefit of mentoring.

8.8. Stress Level (Attention Seeking / Attentiveness)

When learners concentrate their attention on what is being taught the learning is more effective. Thus, it helps in effective teaching learning process. Learning or acquiring any skill is possible only when an individual is attentive while being taught. Moreover, by default, all teachers are attention-seekers.

The statement 'When my students don't pay attention to me, I get upset' shows strong agreeness to the tune of 26.7%, and moderate agreeness also shows the same figure. Therefore, a total of 53.4% have agreed to the above said statement. They are attention seekers. A 13.3% of the respondents have opted for 'neutral' option in the scale. 33.3% of the respondents have disagreed to the above statement which means they don't get disturbed even if the students lack attention. This means they are the teachers who manage the stress situation very well.

8.9. Helping Tendency

Helping others is not only good for those who lend helping hand and a good thing to do. It also makes us happier and healthier too. Doing things for others - whether small, unplanned acts or regular volunteering - is a powerful way to boost our own happiness as well of those around us. Here, the help being offered from the teachers side towards their respective students.

It is to note that around 87% of the respondents have agreed to the statement 'I try to always help my students through difficult times'. This is obvious that being teachers as the second parents of the students have to stand offer helping hand in difficult times. A 6.7% of the respondents have opted for 'neutral' option in the scale and the same percentage of respondents has strongly disagreed to the same statement shown above. This does not mean that these teachers have no botheration about the respective students at difficult times but they may be reluctant to discharge this fatherly role or they may be

willing their students themselves to stand for their own problems and sort them out.

8.10. Relational Happiness

Most of us probably don't believe we need a formal definition of happiness; we know it when we feel it, and we often use the term to describe a range of positive emotions, including joy, pride, contentment, and gratitude. Relational happiness refers to the positive feeling of happiness one enjoys by relating it with some relative action or thing. Here, relational happiness refers to the quantum of happy feeling in teachers which depend on the happy feeling of the respective students.

Eighty percent of the respondents are agreeing to the statement 'I cannot be happy unless I place my students' happiness before my own' which means their happiness is based on the happiness of their own students. These teachers to be happy will always try to keep their wards happy. A 6.7% of the respondents have opted for the option 'neutral' in the scale. The same percentage of respondents have moderately disagreed and strongly agreed, respectively, which means proper orientation is required to these teachers to make them understand the relational happiness concept in their lives.

8.11. Anger Management

Anger is an emotion characterized by antagonism toward someone or something you feel has deliberately done you wrong. Anger can be a good thing. It can give you a way to express negative feelings, for example, or motivate you to find solutions to problems. But excessive anger can cause problems. Anger is a weakness but people think of it as a strength. In actuality, the person who does not display anger has more inner strength than the one who displays it. First, the sparks set you on fire and then you burn others. So, that fire not only hurts you, but hurts others as well.

For the statement 'Whenever any of my students gets angry with me, I still love him/her', 76.6% of the respondents have agreed while only 13.4% have disagreed. A meagre 10% have opted for neutral in the scale. This means using forgiveness as a tool, teachers still shows their love towards their students, in spite of their angriness towards their teachers.

8.12. Endurance

Endurance (also related to sufferance, resilience, constitution, fortitude, and hardiness) is the ability of an organism to exert itself and remain active for a long period of time, as well as its ability to resist, withstand, recover from, and have immunity to trauma, wounds, or fatigue. Endurance here refers to the tolerance or the patience the teachers are experiencing due to their students' behaviours.

For the statement 'I would endure all things for the sake of my students', 76.6% of the respondents have agreed to, while only 13.4% have disagreed. A ten percent of the respondents alone have opted for 'Neutral' option in the scale. This shows that around

3/4th of the teachers having good endurance while 1/3rd of them alone need to develop endurance in them.

9. Findings of the Study

The findings of the study have been presented under ten headings as shown below.

1. Attachment

73.3 per cent of the respondents have strongly agreed that 'Students and they are attached to each other'. A ten percent of the teachers have moderately agreed that they are attached to students. Totally, 83.3% have shown green signal for this attachment statement. Only 6.6 percent of the teachers have shown red signal for this statement that they are not attached to their respective students. Another 10 percent of the students have opted 'neutral' option in the scale which means that they have not tried so for to realise the attachment they have with their students. They are the people who discharge their duty of mentoring just as the task has been assigned to them. They are the people on whom a considerable work needs to be done to develop attachment.

2. Level of Understanding

66.7% of the respondents have strongly agreed the statement 'there is understanding between me and my students'. Similarly, 23.3 per cent of the respondents moderately agreed the above statement. Therefore, totally, 90% of the respondents are having good understanding with their students. 6.7 % of the respondents have opted for Neutral option in the scale which means they are either not ready to understand the opponent or have taken seriously the requirement of understanding between teachers and the students. Only a meagre percentage (3.3) of the respondents have moderately disagree the said statement. These teachers require strong boost to inculcate the habit of developing understanding towards the students. It is very interesting to note that not even a single respondent has selected 'strongly disagree' category that means there is no single teacher who has not at all developed any understanding with the respective students.

3. Expected Intelligence

Here, expected intelligence refers to the level of intelligence students are having. Of course, this is in tune with the expectations of the teachers. The above table shows that a total of 80% of the teachers agreed that the students are up to the expectations of the respective teachers in terms of intelligence. A 10% of the respondents have neutral selection that means either the teachers have not tried to test the students in terms of their intelligence or the students might be shy type that they might not have come forward to show their intelligence. Another 10% of the respondents have opted for 'Moderately Disagree' option and there is none who opted the option 'Strongly Disagree'.

4. Communication

It is interesting note that not even a single respondent opted for 'Neutral' category for the respective statement. That means the respondents are clear with respect to

the statement 'I have no difficulty in communicating with my students'. A total of 93.4% of the respondents are agreeing to the said statement and only 6.6% of them are disagreeing to it. This clearly shows the good communication exist between the mentors and mentees.

5. Friendliness

Seventy percent of the teachers are agreeing to the statement 'I expect to always be friendly with my students' which means these teachers are really expressing friendliness when it comes to dealing with their respective students. 13.3% of the teachers are disagreeing to the above said statement which shows that these teachers are 'strict' kind of teachers who actually do not express their friendliness towards their respective students. Only a 6.7% of the teachers have opted for 'Neutral' option in the scale who are surely those teachers who do not like the concept of mentoring at all.

6. Relationship

Eighty six point seven percent of the respondents are saying that they are satisfied with their respective students when it comes to teacher-student relationship. Only ten percent of the respondents are disagreeing to it. Proper motivation is required to such teachers. A meagre 3.3% of the respondents have opted for 'neutral' option in the scale.

7. Reflection

For the statement 'My main consideration is shaping my students how they would reflect, 50% of the respondents have strongly agreed while 36.7% of them have moderately agreed. Therefore, a total of 86.7% of the respondents have agreed that the mentoring process results in reflection. Students are getting better and better understanding which ultimately results in new learning. It is to note that apart from 13.3% of the respondents who are neutral for the statement, none have disagreed neither moderately nor strongly which means that every respondent except opted for neutral have no doubt about the reflective benefit of mentoring.

8. Stress Level (Attention Seeking / Attentiveness)

The statement 'When my students don't pay attention to me, I get upset' shows strong angriness to the tune of 26.7%, and moderate angriness also shows the same figure. Therefore, a total of 53.4% have agreed to the above said statement. They are attention seekers. A 13.3% of the respondents have opted for 'neutral' option in the scale. 33.3% of the respondents have disagreed to the above statement which means they don't get disturbed even if the students lack attention. This means they are the teachers who manage the stress situation very well.

9. Helping Tendency

It is to note that around 87% of the respondents have agreed to the statement 'I try to always help my students through difficult times'. This is obvious that being teachers as the second parents of the students have to stand offer helping hand in difficult times. A 6.7% of the respondents have opted for 'neutral' option in the scale and the same percentage of respondents have strongly disagreed to the same statement shown above. This does not mean that these teachers have no botheration about the respective students

at difficult times but they may be reluctant to discharge this fatherly role or they may be willing their students themselves to stand for their own problems and sort them out.

10. Relational Happiness

Eighty percent of the respondents are agreeing to the statement 'I cannot be happy unless I place my students' happiness before my own' which means their happiness is based on the happiness of their own students. These teachers to be happy will always try to keep their wards happy. A 6.7% of the respondents have opted for the option 'neutral' in the scale. The same percentage of respondents have moderately disagreed and strongly agreed, respectively, which means proper orientation is required to these teachers to make them understand the relational happiness concept in their lives.

11. Anger Management (by Forgiveness)

For the statement 'Whenever any of my students gets angry with me, I still love him/her', 76.6% of the respondents have agreed while only 13.4% have disagreed. A meagre 10% have opted for neutral in the scale. This means using forgiveness as a tool, teachers still show their love towards their students, in spite of their angriness towards their teachers.

12. Endurance

For the statement 'I would endure all things for the sake of my students', 76.6% of the respondents have agreed to, while only 13.4% have disagreed. A ten percent of the respondents alone have opted for 'Neutral' option in the scale. This shows that around 3/4th of the teachers having good endurance while 1/3rd of them alone need to develop endurance in them.

10. Suggestions

Based on the above findings, the different suggestions for the betterment of mentor-mentee relationship have been made in the following paragraphs.

1. For 10 percent of the students who have opted 'neutral' option in the scale which for attachment statement. They are the people who discharge their duty of mentoring just as the task has been assigned to them. They are the people on whom a considerable work needs to be done to develop attachment.

2. The teachers who disagree with the 'understanding level' statement is required strong boost to inculcate the habit of developing understanding towards the students.

3. Proper motivation is required to teachers to develop satisfactory relationship amongst teachers and students.

4. Opportunities and situations to be created in the work place like cafeteria to not only feed them but also to inculcate and increase the bonding and attachment amidst the teachers and students.

5. It is suggested not to have over expectations for the basic reason that every student is unique in all respects. They have to openly discuss with their respective students about the expectations they have against each one of them, on case by case basis.

6. The teachers have to undergo some short-term course on communication either online or off-line by their own interest or by the intervention of top management or middle management, as the case may be.

7. To imbibe the relevance of friendliness in the work group one-to-one counselling or group counselling can be arranged.

8. Case studies of different fields may be discussed to prove that there is an unparallel role of satisfactory relationship in the work place.

9. The role and the need of reflection in mentor-mentee relationship can be imbibed in the complex minds of these teachers. Many success stories both in the form of articles and video clippings are available on reflection and its benefits in career growth and advancement. They may be circulated among them so as to create a positive approach amidst them towards reflection.

10. Instead of showing upset mood in front of the students on their non-attentiveness, caring attitude is exhibited upon their behaviour, gradually; the students will become attentive.

11. Human-approach based dealings are the need of the hour. The teachers are required to orient towards this. For this purpose, some live examples, from the same institution in which the teacher is working, may be used to boost the morale of the students in this regard.

12. For the statement of happiness, it is suggested to slowly inculcate positivity in the minds of teachers by continuously talking to them about the positivity and its positive impact on one's life. The job may aptly be done by the internal quality assurance cell, if available. In its absence, the management may take the responsibility.

13. Anger Management courses are available online both at free of cost and on payment of prescribed fee, which insist us on proper meditation or diet and offer nice practice whereby one can develop control over his/her anger. The students who have disagreed or kept mum for the anger related statement, need to undergo such courses to develop anger management.

14. By developing the understanding about mentorship, one can develop tolerance and patience. By clear understanding of the expectations of the management from teachers as mentors, they can relate the expectations with the given role and relating the same with the institutional objectives, vision and mission; they can

increase their tolerance level and their patience. Success stories of good leaders worldwide will also help these teachers to develop their tolerance and patience level.

11. Conclusion

Mentorship is no doubt a beneficial thing for any organisational or institutional setup including leather units provided it is carried out with due seriousness and interest. Otherwise, this will also be one amongst others; the absence or presence of which will not bring any considerable change in the set up. Mentorship is an Art which need to be practiced scientifically to get maximum benefit out of it.

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HUMAN RESOURCE AUDIT: A STUDY WITH SPECIAL REFERENCE TO JIO TELECOMMUNICATION SERVICES IN TIRUPATTUR DISTRICT

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Abstract

An audit is a means by which an organization can measure where it currently stands and determine what it has to accomplish to improve its human resources function. It involves systematically review wing all aspects of human resources, usually in a checklist fashion, ensuring that government regulations and company policies are being adhered to. The key to an audit is to remember it is a learning or discovery tool, not a test. There will always be room for improvement in every organization. Auditing, which a part of the control function, may be defined as the examination and evaluation of policies, procedures and practices in all phases of a business to achieve the most effective administration of the organization. In an organization the activities of various departments are constantly reviewed to ascertain if they are moving in the desired direction and to decide what changes should be made in view of altered environmental conditions. In this article, researcher has highlighted the importance of HR Audit towards employees of Reliance Jio.

Keywords: HRM, CEO, HR Audit and JIO.

1. Introduction

Mobile wireless industry has started its technology creation, revolution and evaluation since early 1970. From Mid 1990's the cellular communication industry has witnessed explosive growth. Wireless communication network have become much more pervasive than anyone could have imagined when the cellular concept was first deployed in 1960's and 1970's. Mobile cellular subscribers are increase 40% per year, and by the end of

2010 there will be four times more mobile cellular subscription than fixed telephone line.

The rapid worldwide growth cellular telephone subscribers as demonstrated conclusively that wireless communication is a robust, viable voice and data transport mechanism. The wide spread success of cellular has led to the development of never wireless system and standards for many other types of telecommunication.

2. Human Resource Management - Meaning

Human resource management of employee's skills, knowledge talents, abilities, aptitudes, creative abilities etc. employee in human resource management is treated not only as economic man but also a social and psychological man. Thus, a complete man is viewed under this approach. Employee is treated as a resource. Human resource management is a strategic management function. Employees are treated as profit centre and therefore, invest capital for human resource development and future utility. Organizations are social systems. If one wishes to work in them or to manage them, it is necessary to understand how they operate. Organizations combine science and people, technology and humanity to attain their targets.

Technology is difficult enough by itself, but when you add people you get an immensely complex social system that almost defines understanding. However, society must understand organizations and use them well they are necessary for world peace, successful systems, and other desirable goals that people seek. Modern society depends on organizations for its survival. Human behaviour is unpredictable because it arises from people's deep-seated needs and value systems.

3. Hrm Audit

Human Resource management activity the systematic verification of job analysis and design, recruitment and selection, orientation and placement, training and development, performance appraisal and job evaluation, employee and executive remuneration motivation and morale, participative management, communications, welfare and social security, safety and health, industrial relations, trade unionism, and disputes and their resolution. Human resource is very much useful to achieve the organizational goal and also is a vital tool which helps to assess the effectiveness of human resource functions of an organization.

An audit is a means by which an organization can measure where it currently stands and determine what it has to accomplish to improve its human resources function. It involves systematically review wing all aspects of human resources, usually in a checklist fashion, ensuring that government regulations and company policies are being adhered to. The key to an audit is to remember it is a learning or discovery tool, not

a test. There will always be room for improvement in every organization. Auditing, which a part of the control function, may be defined as the examination and evaluation of policies, procedures and practices in all phases of a business to achieve the most effective administration of the organization. In an organization the activities of various departments are constantly reviewed to ascertain if they are moving in the desired direction and to decide what changes should be made in view of altered environmental conditions.

Besides, in an organization either the top management or the chief executives as the final coordinating agency will want to know how the various units are functioning and how far they have been able to meet policies and guidelines agree upon. The audit may include one division or an entire company. It gives feedback about the human resource functions to operating managers and human resource specialists. It also provides feedback about how well managers are meeting their human resource duties. In short, the audit is an overall quality control check on human resource activities in a division or the entire company and an evaluation of how these activities support the organizations strategy.

4. Objectives of the Study

- To know the effectiveness of human resource functions in the organization.
- To find out the area of improvisation and outcome of the employees upon the application of HRM.

5. Statement of the Problem

HRM can be a challenge for small businesses especially, which typically don't have an HR department to rely on. They may be limited to one HR person, or this responsibility may still belong to the CEO. Regardless, small business owners need to understand the challenges facing them so they're prepared to tackle HR issues as their company, and workforce, grows. As a business grows, its strategies, structure, and internal processes grow with it. Some employees have a hard time coping with these changes. A lot of companies experience decreased productivity and morale during periods of change.

Investing in the training and development of lower-level employees is another common HR problem. Some businesses have trouble finding the resources to do so. Employees on the front lines are some of your hardest workers, and may not have the time to take a training course. The Affordable Care Act has been a pain point for many small businesses in the past few years. Rising healthcare costs mean companies must either pass these costs on to employees, or take a hit to their bottom line. Since good benefits packages can be a deciding factor for potential hires, understanding them is key. Therefore, this study throws light on the important things which have been specified in the objectives.

6. Scope of the Study

Generally, no one can measure the attitude of human being and also their problems are not confined to the Human Resource department alone. So, it is very much broad in nature. It covers the following Human resource areas:

- Audit of all the Human Resource function.
- Audit of managerial compliance of personnel policies, procedures and legal provisions.
- Audit of corporate strategy regarding Human Resource planning, staffing, IRs, remuneration and other Human Resource activities.
- Audit of the Human resource climate on employee motivation, morale and job satisfaction.

7. Review of Literature

The literature on human resource auditing has been described as 'flawed' with the term audit used 'indiscriminately so that almost any kind of study of human resources can be considered an audit' (**Clardy 2004**). In this study the term 'human resource audit' describes the professional practice of auditing applied to human resources management activities, while the term 'review' is used to describe other forms of human resource evaluation.

The word audit comes from the Latin, 'audire' (to listen). Auditing has existed for centuries and can be traced to ancient Egypt, Babylon and Rome. The auditor's role was to 'listen' to the records and the notion of an independent outsider 'looking in' is central to auditing (**Burrowes and Persson 2000**).

8. Research Methodology

The study was conducted through a systematic research work. This study aims to probe into the human resource audit in relation to Reliance Jio. Research is an active diligent and systematic process of enquiry in order to discover, interpret or revise facts, events, behaviours or theories, or to make practical applications with the help of such facts, acts or theories. The sampling design implemented, the process of data collection and the methodology of analysis of the data are explained besides the concept used, limitation of the study are also explained.

9. Research Design

A research design is the arrangement of conditions and analysis of data in a manner that aims to combine relevance to research purposes with economy in procedure. The population of the study comprises of Jio employees of Tirupattur District. From this population, the researcher has stated 150 respondents by following convenient sampling technique. The approach taken for its research is survey method. It was designed in such as to get sufficient information related to the company, human resource department and their functions, effectiveness of human resource functions.

10. Sampling Technique

Sampling technique used in this study is stratified sampling. Population is divided in to 3 strata, on the basis of designations such as managers, supervisors and workers. Then using simple random sampling 30% samples from managers, 20% samples from supervisors and 50% samples from workers had been chosen.

11. Collection of Data

1. **Primary Data:** Primary data were collected through individuals using structured interview schedule and personal interview. Primary data are the original sources from which the researcher directly collected data, in the other words they are first-hand information collected through various method such as interviewing customers, circulation of interview schedule to respondents.
2. **Secondary Data:** Secondary data required for the study has been collected from the annual reports of Telecom Regularity Authority of India (TRAI). The secondary has also been collected from journal, yearbooks of statistics India Telecom Policy, Department of Telecommunication, published report of the world Telecommunication Development, Books and various websites.

12. Data Analysis and Results Discussion

Table 1: Opinion about HR Department is Effective in Delivering Competent Services

Opinion	No. of Respondents	Percentage
True	19	13
Almost True	84	56
Partly True	20	13
Not True	27	18
Total	150	100

Sources: Primary Data

Interpretation

From the above table it discovers that 56% of the workers are agree with this opinion, and 13 % of the workers are partly agree with this opinion.

Hence, the majority (56%) of the respondents comes under the almost true opinion.

Table 2: Opinion about HR Department Manpower Plan is Efficiently

Opinion	No. of Respondents	Percentage
True	23	15
Almost True	77	51
Partly True	46	31
Not True	04	3
Total	150	100

Sources: Primary Data

Interpretation

From the above table it discovers that 51% of the workers are agree with this opinion, 31 % of the workers are partly agree with this opinion and only 3% of the workers are disagreed.

Hence, the majority (51%) of the respondents comes under the almost true opinion.

Table 3: Opinion about HR Department is Accessible to Employees

Opinion	No. of Respondents	Percentage
True	50	33
Almost True	80	53
Partly True	15	10
Not True	05	4
Total	150	100

Sources: Primary Data

Interpretation

From the above table it is clear that most of the employees that is 80workers (53%) are agree with this opinion, 10 % of the workers are partly agree with this opinion and only 4% of the workers are disagreed.

Hence, the majority (53%) of the respondents comes under the almost true.

Table 4: Opinion about Quality Management System is Effective in Achievement its Objectives

Opinion	No. of Respondents	Percentage
True	33	22
Almost True	72	48
Partly True	31	21
Not True	14	9
Total	150	100

Sources: Primary Data

Interpretation

From the above table it is clear that most of the employees that is 72 workers (48%) are agree with this opinion about existing quality management system is effective, 21 % of the workers are partly agree with this opinion and only 9% of the workers are disagreed.

Hence, the majority (48%) of the respondents comes under the almost true opinion.

13. Findings

1. In relation to HR Department is effective in delivering Competent Services, it is found that more than half (56%) of the respondents comes under the almost true opinion.
2. Similarly, the next finding is all about HR Department Manpower Plan is efficiently. In this finding, half of the respondents (51%) comes under the almost true opinion.
3. As regards, HR Department is Accessible to Employees, It is found that majority (53%) of the respondents comes under the almost true.
4. According to Quality Management System, Majority of the respondents positively responded that Quality Management System is effective.

14. Suggestions

Policies should be implemented quickly. Policies refers to policies those which are not implemented by the company until yet. Policies such as Policy on Customer Retention, Feedback Redressal, Quality in Customer Service etc. Such policies are there but not as effective as how they should be in practice. Therefore, the company should throw light on these things so as to enhance the customer base.

Training period should be increased and should be made compulsory to all. There is training in the common schedule of company. But, what matters is period of time, It should be extended in such a way that all the employees get anticipated benefits out of it. Similarly, everyone should undergo training program as and when conducted by the company. Promotion based on performance will motivate the employees to perform better. But they provide promotion on the basis of experience. Performance and Commitment of employees will decided about the promotion of employees. Management should convey the message of promotion to all the employees. Tell the employees of benefits arising out of improving the performance.

15. Conclusion

The study reveals that almost all the functions of the Human resource department is satisfied for top level management that is the managers and supervisors. But lower level workers have more expectations and are not fully satisfied.

Performance management is the area need improvement and at the same way incentives, rewards, training programs and good working condition are few factors which to be improved. This has great impact on employee's performance. We can hope Jio will continue its good performance including the needed changes. The company has to follow the suggestions put forth by the researcher. These suggestions were made keeping in view of ifs and buts witnessed during the findings of the study. The company has to increase the morale among its employees so as to keep them updated, committed and dedicated to the organization.

Training should be cornered as prime importance. Some of the employees are found to be little effective or not effective due to lack of training or ineffective training provided by the organization.

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