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Exploring Identity and Hybridity in Zadie Smith's *White Teeth*

- P. Sophia Morais.*

Abstract

Zadie Smith's fiction eludes literary categorization with its focus on immigration to Britain and development of hybrid identity. In the age of globalization, the issues of diaspora and hybrid identity continuously enrich the diasporic literatures of the twenty first century. Topographical shifting, cultural transactions, multiculturalism, fluid identities form a complex framework in the field of global migration. Recently identity shift in diasporic elements are recurrent themes. Zadie Smith's writings bear the stamp of this identity shift. A mixed culture milieu makes room for vistas of communication and dialogue in this cosmopolitan world. Cultural identities always emerge when the self is dislocated in space and time. This study is an attempt to prove that identity in Zadie Smith's *White Teeth* which is shaped by cultural, racial, linguistic, political and spatial hybridity. It also traces the scope of hybrid identity construction in a multicultural social space using Homi Bhabha's theory. The critical theorist, Homi K. Bhabha has put forth the key concepts of mimicry, difference and ambivalence. Bhabha is the most important critic connected to the term Hybridity, which means joining of two entities to form a new entity. He views hybridity as a type of 'third space'. The 'third space' enables new structures to emerge by displacing history and past culture to form a new culture. With an incredibly realistic portrayal of human nature, *White Teeth* celebrates the 'third space' by portraying a forceful representation of space in the modern city London.

Keywords: Diaspora, Multiculturalism, Assimilation, Hybrid Identity, Third Space, Homi Bhabha's Theory.

In contradiction to essentialist ideology, the concept of identity in a multicultural society is regarded as an ever changing process of construction and enactment. Stuart Hall says that "the construction of one's identity is affected by political, historical and social dimensions as well as personal ones" (*Identiteetti* 6). Societies, which are forms of cultural power, affect an individual's construction of identity. So a mixed culture makes room for hybrid identities in a multicultural society. The concept of hybridity denotes the joining of two entities to create a third entity.

In Zadie Smith's *White Teeth* people move across national borders and adopt the new cultural identities forming new hybrid identities. "Bhabha contends that cultural statements and systems are constructed in a space that he calls the 'Third Space of enunciation'" (*Post-Colonial Studies* 118). Cultural identities always

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emerge when the self is dislocated in space and time. "It is the 'in - between' space that carries the burden and meaning of culture, and this is what makes the notion of hybridity so important" (*Post-Colonial Studies* 119). This study will attempt to prove that identity in Zadie Smith's *White Teeth* is shaped by cultural, racial, linguistic, political and spatial hybridity. It also traces the scope of hybrid identity construction in a multicultural social space using Homi Bhabha's theory.

Zadie Smith's *White Teeth* presents Britain as a diverse and multicultural society. The pivotal focuses of the novel are three families - the Jones', the Iqbals and the Chalfens. Though all the three families are of mixed ethnicity, culture and religion, they create a sense of Britishness and a sense of belonging in the city of London. So the characters are the embodiment of hybridity and cultural diversity. The spatial dimension thus becomes prominent in the novel and this space as a hybrid location is an inherent part of the modern British society. Bhabha says that "it is to the city that the migrants, the minorities, the diasporic come to change the history of the nation . . . it is the city which provides the space in which emigrant identifications and new social movements of the people played out" (*The Location of Culture* 243).

The New Empire is undergoing a critical phase in its post-colonial period. It is the crisis of the entire society where "culture-as-hegemony is the malleable, transparent, power-laden glue holding together- and lubricating-the different spheres and strata of society. In effect culture is the very stuff of which individual and collective identities are made" (Hussein175). Cultural identity manifests itself in the individual's search of personal identity. Stuart Hall points out two kinds of cultural identities. In the first he "defines 'cultural identity' in terms of one, shared culture, a sort of collective 'one true self', hiding inside the many other, more superficial are artificially imposed 'selves', which people with a shared history and ancestry hold in common" ("Cultural Identity and Diaspora" 435).

Here Stuart Hall speaks about commonality that is searching for one's roots. "Culture is the combination of motor and mental behaviour patterns arising from the encounter of man with nature and with his fellow man" (Haddour 19). Cultural identities are generally historical experiences and mutual cultural codes. This concept of cultural identity played a vital role in reshaping the globe. Such identity is not grounded in the archaeology but in hunting for the origin.

In *White Teeth* the characters of mixed ethnicity tussle with the issues of heritage and legacy. The first generation character Samad Iqbal, the Bangladeshi has internalized the cultural codes of London without getting rid of his heritage and ancestry. Samad clings to his past exhibiting the Oriental cultural heritage. Samad's religion has a great impact in his life and this is evident from these words, "Nobody even thinks to pick up the Qur'an. Key item in an emergency situation: spiritual support" (222).

Samad wants his son Magid to be brought up in his Bengali Muslim roots and accomplish his great-grandfather Mangal Pande's legacy of devotion to his nation. For this purpose he kidnaps his own son Magid and sends him to Bangladesh. But this does not prevent the second generation Magid from becoming an English intellectual. Samad pours his feelings of the two cultures, "That is precisely the point! I don't wish to be a modern man! I wish to live as I was always meant to! I wish to return to the East!" (145).

Irie is the character most frustrated by her roots. Irie is born of a British father and a Jamaican mother. She hates how the past and the cultural heritage complicate her existing life. Therefore, she feels deceived when she finds out that Clara's upper teeth are false. So in order to discover her roots, she seeks the help of her maternal grandmother Hortense Bowden.

According to Stuart Hall the second kind of cultural identity recognizes that there are many critical points to fathom the significant differences "which constitute 'what we really are'; or rather-since history has invented-'what we have become'. We cannot speak for very long with any exactness about 'one experience, one identity', without acknowledging its other side-the ruptures and discontinuities" ("Cultural Identity and Diaspora" 435). Here Stuart Hall speaks about the newly formed identity which keeps on changing. This second kind of identity belongs to the future, crossing across the limits of place, time, history and culture. Through this second form we can identify the disturbed character of the colonial experience. The influence of the British culture is prominent in the Jamaican woman Clara. Clara undergoes a continuous process of transformation and her identities are fluid. So her identity and the space she inhabits are not fixed and homogeneous but pliable and heterogeneous. Smith

skilfully uses the metaphor of teeth to represent Clara's fluid identity. "When Clara fell, knocking the teeth out of the top of her mouth, while Ryan knew it was because God had chosen Ryan as one of the saved and Clara as one of the unsaved" (44).

In the scooter accident Clara loses her upper teeth. This metaphorically shows that she is rejecting the Jehovah's Witnesses, breaking her relationship with Ryan Topps and losing her Jamaican identity to form a new identity. Clara's identity is highly assimilative, she can easily adopt and accommodate to her newly settled British culture. She travels through a hybridized space where the novelist constructs the notion 'in-betweeness'. Edward Said "insists that all cultures are changing constantly, that culture and identity themselves are processes" (*Edward Said* 5).

The character Magid, the Bangladeshi holds an English identity. Magid is sent to Bangladesh to become a devout Muslim. But he returns to England "more English than the English" (406). Magid is transformed as an English intellectual because of his encounter with the Indian writer Sir R.V. Saraswathi. He taught Magid that "Too often we Indians, we Bengalis, we Pakistanis, throw up our hands and cry "Fate!" in the face of history. But many of us are uneducated; many of us do not understand the world. We must be more like the English. The English fight fate to the death. They do not listen to the history unless it is telling them what they wish to hear" (288).

Magid's geographical border crossing ironically led him to adopt English identity. Since Bangladesh is a part of the English colonies, Magid returns from his Orient land as "a pukka Englishman, white suited, silly wig lawyer" (407). Thus Magid thrives with an identity of an Oriental British. In their displacement and diverse experiences Bhabha says in his *Location of Culture* that "the borders between home and world become confused and, uncannily, private and the public become part of each other, forcing upon a vision that is dividing as it is disorientating" (1). This disorientation becomes still more visible when Magid joins hand with Marcus Chalfen who is "more English than the English" (328). Thus cultural identities are the points of a person's identification.

The next part of this study attempts to analyse Hybridity which is the joining of two entities to form a new entity. Homi K. Bhabha is the most important critic connected to the term hybridity. He views hybridity as a type of 'third space'. The 'third space' enables new structures to emerge by displacing history and past culture to form a new culture. Bhabha redefines "culture discourse, and identity as fluid and ambivalent, rather than fixed and one dimensional. While emphasizing the hybridity of all cultures, Bhabha closely links the notion of hybridity to the spatial metaphor of the third space, a concept that is inspired by the works on spatiality by historians and philosophers" (Acheraiou 90).

Ashcroft says that hybridity is an outcome of "new transcultural forms within the contact zone" (Post-Colonial Studies 118). It is often the result of colonialism. The contact zone is created between two or more cultures in which hybridization emerges in many forms like cultural, racial, linguistic and political. Hybridity has often been used in post-colonial discourse to mean cross-cultural exchange. Bhabha calls this cross-cultural exchange as 'Cultural Hybridity'. Here he connects the notion of cultural hybridity to the spatial metaphor of the 'third space'. He says that the third space is interchangeable with hybridity. Bhabha further states:

> All forms of culture are continually in the process of hybridity. But for me the importance of hybridity is not to be able to trace two original moments from which the third emerges, rather hybridity to me is the 'third space' which enables other positions to merge. . . . The process of cultural hybridity gives rise to something different, something new and unrecognizable, a new area of negotiation of meaning and representation. (*The Location of Culture* 211)

With an incredibly realistic portrayal of human nature, *White Teeth* celebrates the 'third space' by portraying a forceful representation of space in the modern city London. Smith's characters are caught between two or three cultures. Millat is trapped between honouring his parents' heritage and in exploring the Western pop culture. Millat becomes a member of KEVIN, a combative fundamentalist of Islamic nation in order to fulfil his passion to become a Western gangster. He is caught between Oriental and Occidental cultures. "Cultural experience and cultural forms are radically, quintessentially hybrid claims, Said" (*Edward Said* 93). Millat inhabits an in-between space where he lives in a space of uncertainty. He moves from one space of social interaction to another space of social seclusion.

In the same way Millat's father Samad Iqbal is also caught between two cultures. Samad who is much concerned with his Muslim Bengali tradition also cannot escape from the in-between space created by the western culture. He is caught between his Islamic faith and his passion for the music teacher, Poppy. "Samad closed his eyes and heard the words,' To the pure all things are pure and then, almost immediately afterwards Can't say fairer than that. Samad opened his eyes and saw quiet clearly by the bandstand his two sons, their white teeth biting into two waxy apples, waving, smiling" (182).

Magid and Millat caught sight of their father Samad with their music teacher Poppy as they bite the apples with their white teeth. Smith uses the metaphor molars to reflect that the twins are able to digest their father's action with another woman and therefore they are destined to follow in his footsteps. From this it is visible that the characters travel in a multicultural space. The spatial dimension is the most important factor in a multicultural society because spaces are the ongoing process of change and newness.

Irie is another figure of cultural hybridity. She despises how the past and cultural heritage complicates and restricts her present life. It is in this context, Irie gets associated with the white Chalfen's family to become completely British.

> The result is a characteristic 'hybridity', or 'in-betweeness', greater than or at least different from some of its colonizing and colonized parts. In so far as the colonizing power attempted to 'reform' the subjectivity of its colonized subjects, what Bhabha calls colonial 'mimicry' became central to the form of hybridity: an 'ironic compromise' between domination and difference, which produced an Other that is almost, but not quite the same. Mimicry is thus the sign of the double articulation. (Milner 146)

This colonial mimicry is seen in the character Irie. She imitates the white Chalfen's who are scientifically oriented and their focus is only on the present and future. Like them Irie too just wants to look forward on future, "when roots won't matter more because they can't because they mustn't because they're too long and they're too torturous and they're just buried too damn deep" (527). In order to become completely British, Irie follows the white in her dress codes and behaviour. The instance of Irie straightening her curly hair to look like a white is highlighted as a mockery in this context. Bhabha says that when the colonized 'Other' imitates the colonizer then that imitation is called a colonial mimicry and has an element of mockery in it.

Secondly, Bhabha speaks about 'Racial Hybridity'. Race or racism is a biologically constructed reality. In Britain the Whites established their racial superiority over the non-whites. Slave sexual oppression steadily increased the degree of hybridity in Britain. Smith highlights this process of change through the story of the Jamaican black woman, Ambrosia.

> The black/white dichotomy remains at the very centre of 'race' discourse whether or not, and to whatever extent, 'race' is explicitly biologized are seen as an essential human property. The distinctive connotative properties of 'black' and 'white' maintain power and material reality, and it would be an act of disavowal to deny the significance of the visible markers of racial identity in contemporary Britain. (Acheraiou 135)

Hortense Bowden is the daughter of a White English officer, Captain Charlie Durham and his Jamaican black maid Ambrosia. Hortense is a hybrid fruit of a forced relation. Smith recalls the past act of slavery in her novel. She writes that when captain Durham was posted to Jamaica, he made his black slave Ambrosia pregnant with a child. Ambrosia's child Hortense is a figure of racial hybridity. This hybridity is the result of a contaminated encounter and space. Smith expresses the indeterminate state of Ambrosia in a new space saying.

> Early will I seek thee . . . my soul thirsteth for thee . . . . So sang Ambrosia as her pregnancy reached full term, and bounced with her huge bulge down King Street, praying for the return of Christ or the return of Charlie Durham – the two men who could save her – so alike in her mind she had the habit of mixing them up. She was half way through the third verse . . . when that rambunctious old rum pot Sir Edmund Flecker Glenard, flushed from one snifter too many at the Jamaica Club, step into their path. Captain Durham's maid! (360)

Smith next talks about the story of Hortense's daughter Clara Bowden. The Jamaican girl Clara and the English Archie Jones fell in love and are brought together in marriage. This happens not in Jamaica but

in England which says about one's free will to choose their partners in a space established in modern Britain. This portrays the present multicultural England formed between the generation gap and the in-between space created. Ambrosia's story and Clara's story exemplifies the shift from a forced hybridity in Jamaica to a desired hybridity in Britain. Ambrosia was pregnant under forced conditions by Captain Durham but on the other hand Clara was pregnant through her legal marital life with her husband Archie.

The novel then focuses on Irie Jones, the pivotal hybrid figure of the younger generation. She is a figure of racial and cultural hybridity born of a black Jamaican – English mother and a White English father. Irie becomes a still more complicated figure of hybridity when she conceives a child with Magid or Millat. Even a paternity test cannot tell whether her child's father is Magid or Millat, since their genes are identical. Irie gives birth to a daughter who is a problematic mixture of three races – the Jamaican, the British and the Bangladeshi. The biological paternity of the baby will be unidentified forever. But the baby will be brought up by Irie and Joshua, with whom Irie fell in love at the end.

Smith herself in an interview said that the novel is a utopian view of race relations. The growing racial multiplicity in contemporary Britain is carefully studied by Smith in her novel *White Teeth*. Assimilation of the characters to new culture results in wide variety of racism. Bhabha says that the central notion of racial hybridity is the International culture which is located in the in-between space of translation and in a continuous negotiation of meaning and cultural identities.

Next, this study attempts to analyse 'Linguistic Hybridity' which is an intermixing of two languages. Language functions as a force in Zadie Smith's *White Teeth*. Today every nation is linguistically hybrid. Colonialism has paved a way to learn the colonizers language and has resulted in linguistic intermixing. This linguistic intermixing is intensified in a multicultural society.

A day to day example of linguistic hybridity is clearly visible in Millat's use of language. Millat and his friends speak a hybrid mix of various languages. Smith states that it is a "strange mix of Jamaican patois, Bengali, Gujarati and English" (231). Millat's use of language is completely different from Archie's manner of speaking. Archie speaks humorously in an old fashioned way. Archie uses comical phrases like "I should cocoa!" (120). It ironically means that he should say so.

Linguistic hybridity can also be seen at O'Connell's Pool House. It is a pub where Archie and Samad often meet. It is a place of diverse cultural mix. The walls are carpeted with "George Stubb's racehorse paintings, the framed fragments of some foreign, Eastern script" (183). The wall was also decorated with "an Irish flag and a map of the Arab Emirates knotted together and hung from wall to wall" (183). This decoration binds together all the cultural elements of the Occident and the Orient and hybridizing them.

Another fine example for linguistic hybridity is the name of the owner of the pub. He is an immigrant named Abdul-Mickey. His name is a combination of Arabic and English words. This hybridized name was born out of two linguistic cultures. Also Abdul agrees to hang the portrait of Samad's great grandfather Mangal Pande. The word Mangal Pande is very astonishing to be heard in a Muslim family. It is a name related only to the Hindus. From this it is clear that Smith's novel is completely against purity and it is constantly speaking about mixed hybridity. Even names which are linguistically hybrid have evolved in the in-between space. "There is substantial evidence that intense mutual cultural and linguistic exchanges occurred through the proximity of colonizers and colonized cultures" (Acheraiou 18).

Power structure is another prominent feature visible in Zadie Smith's *White Teeth.* The term hybridity was much influential in the imperial and the colonial discourse. Ashcroft says that "post-colonial theory investigates, and develops propositions about, the cultural political impact of European conquest upon colonized societies and the nature of those societies' responses" (*Edward Said* 15). *White Teeth* depicts a dynamic image of the city of London. It allows the characters to collaborate and produce different spaces. Bhabha states:

> Third space displaces the histories that constitute it, and sets up new structures of authority, new political initiatives, which are inadequately understood through received wisdom. . . . The process of cultural hybridity gives rise to something different, something new and unrecognizable, a new

area of negotiation of meaning and representation. (*Nation and Narration* 211)

The concept of power structure can be traced in the novel through the life of the character Samad Iqbal. Samad was easily transferred from the Indian army to the new space, the English army because of Britain's connection with India. During World War II, Britain was in need of labours and so it encouraged immigration. Thousands of Italians and Poles were imported but still there was shortage and the British marched towards the West Indies. As a result many West Indians, especially Jamaicans landed in London. This gave rise to much political diversity in the contemporary London.

Smith skilfully lays out three different manifestations of political structures established as an outcome of the space evolved through migration. The novel casts light on three political movements - KEVIN, FATE and FutureMouse.

KEVIN refers to 'Keepers of the Eternal Victorious Islamic Nation'. Millat quits his love for western pop culture and becomes a member of this Islamic fundamentalist group. KEVIN and FutureMouse ignite combat between the twins. Millat refuses to see his twin brother Magid because he supports FutureMouse which Millat protests. A varying political space is created between the members of the same family.

The next issue which the novel focuses is the 'FATE'. It is a political movement 'Fighting against Animal Torture and Exploitation'. FATE was founded and run by Joely and her husband Crispin. Joshua and other members of FATE are involved in the animal cruelty abolishing work just to get closer with Joely. Therefore many members of KEVIN and FATE are more interested in gaining a political status and the thrill of fundamentalism than in its doctrine. Thus many characters are displaced and transformed in the spatial confguration.

The most highlighted political concept in *White Teeth* is the FutureMouse. It is Marcus Chalfen's highly controversial experiment. It is a genetic engineering research with a mouse in which he has altered a mouse's genes to develop cancer at specific times in its life. Chalfen hopes that this research might someday help to cure cancer. Here the political hybridity is much clearer – FutureMouse experiment creates cancer in order to cure cancer. Duality emerges in the third space. That is, on one hand FutureMouse creates cancer in the mouse and on the other hand FutureMouse cures cancer patients.

In the chapter 'The Final Space' all the characters of the novel gather to witness Professor Marcus' experiment. The space created here is referred as "new British room, a space for Britain, Britishness, space of Britain, British industrial space cultural space" (518). The people who live in this century are "forced from one space to another . . . renamed, rebranded, the answer to every questionnaire noting nothing space please just space nothing please nothing space" (518-519). All these prove that despite plurality, differences and diversity, there is a common space for the British society. Whether black, white or brown Britain has a 'third space' to exist.

The novel beautifully portrays a multicultural space where heterogeneous identities are formed. *White Teeth* is a powerful display and vibrant representation of the spaces in the hybridized British society which celebrates the "third space'. Smith's fiction is a brilliant construction of hybrid reality in an ethnically diverse nation. This study of Zadie Smith's *White Teeth* thus demonstrates that identity in the novel is shaped by cultural, racial, linguistic and spatial hybridity. This construction of hybrid identities takes place in a multicultural space. Therefore the novel is a manifestation of both identity and hybridity.

Bibliography

Primary Source

1. Smith, Zadie. *White Teeth*. London : Penguin Books, 2000. Print.

Secondary Source

1. Acheraiou, Amar. *Questioning Hybridity, Postcolonialism and Globalization*.
2. UK: Palgrave Macmillan, 2011. Print.
3. Ashcroft, Bill, Gareth Griffith, and Helen Tiffin. *Post-Colonial Studies: The Key Concepts*. London: Routledge, 2000. Print.
4. Ashcroft, Bill, and Paul Ahluwalia. *Edward Said*. 2nd ed. London: Routledge, 2001. Print.
5. Bhabha, Homi K., ed. *Nation and Narration*. London: Routledge, 1990. Print.
6. - - - , *The Location of Culture*. London: Routledge, 1994. Print.

7. Haddour, Azzedine, ed. *The Fanon Reader: Frantz Fanon*. London: Pluto Press, 2006. Print.
8. Hall, Stuart. "Cultural Identity and Diaspora." *The Post-Colonial Studies Reader*. Eds. Bill Ashcroft, Gareth Griffth, Helen Tiffin. 2nd ed. London: Routledge, 1995. Print.
9. - - - , *Identiteetti*. Trans. and Ed. Lehtonen M. and J. Herkman. Tampere: Vastapain,1999. Print.
10. Hussein, Abdirahman A. *Edward Said: Criticism and Society*. London: Verso, 2002. Print.
11. Milner, Andrew, and Jeff Browitt, eds. *Contemporary Cultural Theory*. 3rd ed. Jaipur: Rawat Publications, 2003. Print.

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Quality of Work Life of Employees: Emerging Dimensions

- Dr. L. Santhana Raj*

Abstract

Many factors determine the meaning of Quality of Work Life (QWL), one of which is work environment. QWL consists of opportunities for active involvement in group working arrangements or problem solving that are of mutual benefit to employees or employers, based on labor management cooperation. This article reviews the meaning of QWL, analyses dimensions of QWL, practices of QWL, techniques for improving QWL and judgment methods of QWL in an organization. The dimensions of QWL include health and well-being, job security, job satisfaction, competence development and the balance work and non-work life.

Keywords: Quality of Work Life, Job satisfaction, Work life and Non work life balance, career development, Job involvement.

Introduction

Human resources play a very important role in success of an organization and thus management of human resources. One such aspect is quality work life [QWL]. It is a philosophy, a set of principles which holds that people are the most important resources in the organization as trustworthy responsible and capable of making valuable contribution and they should be treated with dignity and respect. The elements that are relevant to an individual's quality of work life include the task, the physical work environment, social environment within the organization system and relationship between life on and off the job.

QWL means "the degree to which members of a work organization are able to satisfy important personal needs through their experience in the organization." QWL has gained deserved prominence in the organizational behavior as an indicator of the overall human experience in the work place. It plays a key role in any organization and has an effect on the people, their work performance and self development; it basically refers to relationship between the employees and ecosystem in which he works. It focuses on creating a working environment where employees work co-operatively and achieve results collectively.

Meaning and Concept of QWL

The term quality of work life has different meanings for different people; some consider it industrial democracy or code termination with increased employee participation in the decision making process. For others particularly managers and administrators, the term denotes improvement in the psychological aspects of work to Improve productivity. Unions and

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workers interpret it as more equitable sharing of profits, job security and healthy and human working condition. Others view it as improving social relationship at work place through outcomes, workgroups. Finally some others take a broader view of changing the entire organization climate by humanizing work, individualizing organizations and changing the structural and managerial system. QWL refers to the quality of relationship between employees and the total working environment. According to Harrison, QWL is the degree to which work in an organization contributes to material and psychological well-being of its members. One expert defines quality of working life as a process of joint decision making, collaboration and building mutual respect between management and employees. It is concerned with increasing labor management co-operatives to solve the problems of improving organizational performance and employee satisfaction.

The concept of QWL is based on the assumption that a job is more than just a job. It is the center of a person's life. In recent years there has been increasing concern for QWL due to several factors:

1. Increase in education level and consequently job aspirations of employees;
2. Association of workers;
3. Significance of human resource management;
4. Widespread industrial unrest;
5. Growing of knowledge in human behavior, etc.

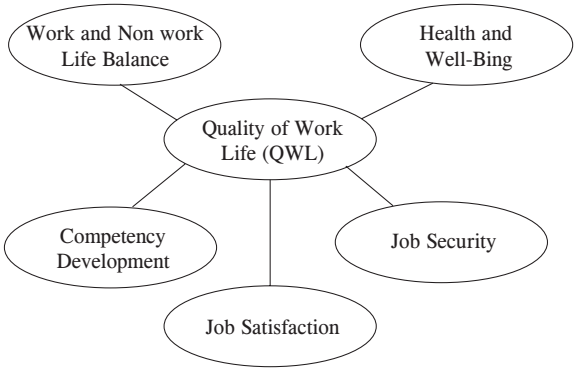
Objectives of QWL

The results, reported from a number of qualities of work life improvement programmes, have some common characteristics. These are:

1. Persistent commitment from management to the open non-defensive modus operandi of sincerely inviting collaborative inputs from the workforce regarding problem identification and suggestions for improving any aspect of the organization or the policies, practices and structure of work with incentives provided for such participation.
2. Invited involvement of members of tasks groups in recommending resolution of identified problem.
3. Training of supervisors to prepare them to function effectively in a less authoritative style.
4. Implementation of practicable suggestion and explanations for rejected ideas.
5. Feedback and recognition for good results achieved.
6. Selection of personnel who can be motivated under appropriate conditions to strive for excellence in task performance.
7. Evaluation and analysis of results, including failures, leading to renewed effort towards continual improvement in modus operandi.

Dimensions of Quality of Work Life

The dimensions of QWL are health and well-being, job security, job satisfaction, competence development and the balance between work with non-work life. Each of the dimensions of QWL from the perspectives of employees is briefly discussed below.



Health and Well-Being

Health and well-being of QWL refer to physical and psychological aspects of an individual in any working environment. Asakura and Fujigaki(1993) Asakura and Fujigaki (1993)7 examined the direct and indirect effect of computerization on workers health and well-being. Their results were similar to the study of Lacovides, Fountoulakis and kaprins (2003)7 that higher job demand leads to higher strain work environment, hence; it affects their health and well being. An unstrained work environment ensures good health and psychological conditions which enable the employees to perform job and non-work related functions without inhibitions. Thus, it leads to an un-stressful work environment providing comfortable

work life. There are many definitions of stress as it is deemed as a subjective phenomenon of QWL. Physical illness and psychological disorders increase when pressure at work increases. Stress causes problems to the muscular system and circulation thus, increasing the risk of myocardial which is well documented in psychosomatic studies.

Job Security

A dramatic change of workforce in contemporary work environment has revealed a significant amount of organization change (Watson *et al*., 2003)11. Organization change such as downsizing, rightsizing and outsourcing have adversely affected employees' loyalty, morale, motivation and perceived job security. Organization of Economic Cooperation and Development (OECD) (1996)12 highlighted that job security is the most controversial issue in contemporary work environment. Job security, the central aspect of QWL represents strength of the organizations to provide permanent and stable employment regardless of the changes in work environment. Hence, providing a sense of security is important especially in the work environment where many facets of jobs can be outsource.

Job Satisfaction

Later, cognitive and behavioral components were added to this definition. The cognitive aspect represents an employee's belief about his job situation. This means an employee may believe that his or her job is interesting, stimulating, or otherwise. The behavioral component represents an employee's behavioral tendencies toward his or her job. The action of attending work regularly, working hard and intending to stay in the organization for long period of time shows the positive behavior which indicates job satisfaction. In contrast, negative behavioral outcomes reveal dissatisfaction in job. Job satisfaction of an employee differs in meaning and importance in relations to the facets of work. Some may feel pay and fringe benefits that meet their expectations to be extremely important for another, it may be essential to have a job that provides an opportunity for challenging assignment. The results of previous studies indicate that many different aspects of the job, such as pay, promotions, supervision, fringe benefits, one's co-workers' support, and excessive working hours(Watson et al,. 2003) are associated with level of satisfaction.

Competency Development

Growth in skills and knowledge is an important aspect of competency development that enhances QWL. Therefore competency development is operational zed as the nature of the job that provides opportunities and stimulates growth in skills and knowledge either for career of organizational development. Career development opportunity will provide essential Training that will help the individual employees to equip with the new skills to spearhead in their career. Most contemporary organizations do not limit themselves to just training an employee for a job, but they go beyond to furnish them with a support system that encourages workplace learning.

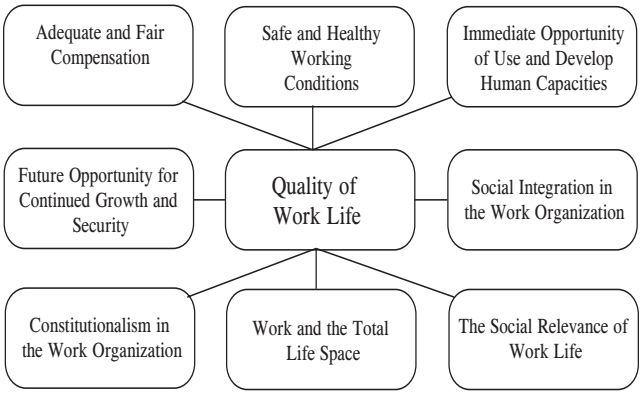
Learning opportunities and skill discretion have also proven to have a positive effect on job satisfaction and reduced job stress that will lead to better QWL. The opportunity to develop and the use of skills are associated with learning mechanisms. This applies especially when the job requires employees to deploy cognitive skills. In contrast, high job demands with inadequate control reduce the ability and opportunities to develop new skills and knowledge and thus enforce negative attitudes and anxiety which deteriorate QWL.

Work and Non-Work Life Balance

A major component of QWL, which is important for both the employees and the employers, is the relationship between work and home life. In an increasing competitive environment, it is difficult to separate home and work life. Employees today are more likely to express a strong desire to have a harmonious balance among career, family life and leisure activities. Organizations need to provide alternative means of employment practices to eliminate the pressure of spillover without influencing the career progression. The balance is important particularly among the employees in order to nurture and develop the sustainable human resource practices in the work environment. Therefore, balance between work and non-work life is suggested as one of the measures of QWL.

Practices of QWL

Quality of working life though came into circulation in 1970s became popular only in 90s and an organization realized its potential to enhance the productivity in the new century. This works as a comprehensive model to those employers who want to ensure quality in working life of their employees. Walton (1973)16 proposes an ideal quality of work life programme will include practices in eight major areas as discussed below;



Adequate and Fair Compensation

This is fundamental to QWL. Human beings work for livelihood. Therefore success of rest of the initiatives depends upon fulfillment of this. However, important here is that compensation offered must be adequate implying it must be proportionate to labor, and there should be internal consistency among salaries of employees.

Safe and Healthy Working Conditions

Unsafe and hazardous working conditions cause problems to both employers and employees. There may be little advantage to the employer in short-term but in medium and long-terms, it adversely affects the productivity. Therefore, adequate investment must be made to ensure safe and healthy working conditions.

Immediate Opportunity of Use and Develop Human Capacities

The works have become routine, meaningless and too specialized, depriving the employees of fulfillment and satisfaction. Therefore, efforts should be made to increase the autonomy, perspective and exposure to multiple skills.

Future Opportunity for Continued Growth and Security

This is related to career aspects of employees. Meaningful career paths must be laid down and career mapping of employees is to be followed. The provisions of advancement opportunities play a central role in QWL.

Social Integration in the Work Organization

Relationships between and among the employees is an indicator of healthy work organization. Therefore, opportunities must be provided for formal and informal interactions. All kinds of religion, races, crafts, and designations must be treated equally on a social platform. In other words, it creates egalitarian environment.

Constitutionalism in the Work Organization

This is related to organizational norms that affect the freedom of an individual employee. Efforts must be made to make sure that right norms are formed in the organization. It means norms that accommodate the privacy of an individual employee, freedom of speech, equity and freedom to dissent on some aspects.

Work and the Total Life Space

Employees should not be allowed to continuously exert themselves. The continuous hard work causes psychological and physical strains. Therefore, there has to be a balance between personal and professional life. Organization must create proper work offs to enrich the life of employees.

The Social Relevance of Work Life

Employees must be given the perspective of how his/her work in the organization helps the society. This is essential to build relevance of the employee's existence to the society he/she lives in.

Techniques for Improving Quality of Work Life

The quality of work life movement is of recent origin and has a long way to go. Individuals as well as

organized efforts are required to improve the quality of work life for millions of workers in the country. In 1981 the National Productivity Council organized a national seminar on quality of work life. The seminar made several suggestions and pointed out the responsibilities of different groups such as employees, unions and workers, professional organizations, and government etc, in improving the quality of work life. Some of them are:

1. Job Redesign
2. Career Development
3. Autonomy
4. Flexible Work Schedules
5. Participative Management
6. Job Security
7. Administrative Justice.
8. QWL and Management Role

QWL and Judgment Methods

The following indices may be used to judge the quality of work life in an organization:

Job Satisfaction

It implies the worker's satisfaction with the environment of his job environment consisting of nature of work, quality of supervision, pay, coworkers, opportunities for promotion, etc. Job satisfaction is related to job involvement and people involved in job are satisfied with their jobs and vice versa.

Sense of Competence

It refers to the feeling of confidence that an individual has in his own competence. Sense of competence and job involvement reinforce each other. When an individual acquires a greater sense of competence he becomes more and more active in work activities. When he feels more competent he becomes more involved in job and becomes better motivated.

Job Performance

When an individual's job involvement, job satisfaction and sense of competence increase, there is a rise in job performance.

Productivity

When the level of job performance increases the output per unit of input goes up. Thus, match between job characteristics and productivity traits of employees generally result in higher productivity.

Conclusion

Quality of Work Life (QWL) is a comprehensive phenomenon that includes an individual's job related well-being and the extent to which work experiences are rewarding, fulfilling and devoid of stress and other negative personal consequences. The QWL has been increasing several factors. These include increase in education level and consequently job aspirations of employees association of workers; significance of human resource management; widespread industrial unrest; growing of knowledge in human behavior, and the like. The elements of QWL comprise of health and well-being, job security, job satisfaction, competence development and the balance between works with non-work life. In this context, for improving the QWL different groups have taken responsibility such as employers, workers, professional organizations, government and managers, leading to quality circles, management by objectives, suggestion system and other forms of employees' participation in management that help to improve QWL in the industry circles. Techniques to improve quality of work life include job redesign career development, flexible work schedules, job security and the like. If any organization properly adopts these techniques, the QWL will certainly be improved to the desired levels.

References

1. Straw, R.J. and C.C. Heckscher, 1984. QWL: New working relationships in the communication industry. Labor Studies J., 9, pp 261, 274.
2. Cunningham, J.B. and T. Eberle, 1990. A guide to job enrichment and redesign. Personnel, 67, pp 56, 61.
3. Feuer, D., 1989. Quality of work life: a cure for all ills? Training: The Magazine of Human Resources Development, 26, pp 65, 66.

4. Walton, R.E., 1975. Criteria for Quality of Working Life. In L.E. Davis, A.B. Cherns and Associates (Eds.) the Quality of Working. New York: The Free Press, Life, 1, pp 91,104.
5. Shamir, B. and I. Salomon, 1985. Workathome and the quality of working life.Acad. Manag., 10: pp 45, 54, 64.
6. Davis, L.E. "Leaerning from the Design of New organisation" in H.F Kolodny and H.Van Beinum (eds.), the Quality of Working Life and the 1980s, New York: Praeger, 1983.
7. Asakura, R., & Y., Fujigaki, 1993. "The Impact of Computer Technology on Job Characteristics and Worker Health". In: M.J. Smith and G., Salvendy (ed.) Human Computer Interaction: Applications and Case Studies, New York: Elsevier, pp 982, 987
8. Iacovides, A., K.N., Fountoulakis, G.K., St. Kaprins, 2003. "The Relationship between Job Stress, Burnout and Clinical Depression". Journal of Affective Disorders, 75, pp 209, 221.
9. Chan, K.B., G., Lai, Y.C., Ko, and K.W., Boey, 2000. "Work Stress Among Six Professionals Groups: The Singapore Experience". Social Science and Medicine, 50, pp 1415, 1432.
10. Carayon,P.,M.C.,Haims,andS.,Kraemer,2001. "Turnover and Retention of the Information Technology Workforce: The Diversity Issue". In: Smith M.J. and G., Salvendy, eds Systems, Social and Internationalization Design Aspect of HumanComputer Interaction. Mahwah, NJ: Lawrence Erlbaum Associates, pp 67, 70.
11. Watson, I., J., Buchanan, I., Campbell, and C., Briggs, 2003. "Fragmented Futures: New Challenges in Working Life". Sydney, New South Wales: The Federation Press. Organization of Economic Cooperation and Development, 1996. "Technology, Productivity and Job Creation", 1 & 2, OECD, Paris.
12. Scully, J., A., Kirkpatrick, and E., Locke, 1995. "Locus of Knowledge as a Determination of the Effects of Participation on Performance, Affect, andPerceptions". Organizational Behaviour Human Decision Making Process, 61, pp. 276, 288.
13. Lewis, S. 1997. "An International Perspective on Work Family Issues". In: S.Parasuraman and J.H. Greenhaus eds Integrating Work and Family: Challenges and Choices for a Changing World. Westport, CN: Quorum Books.
14. Aminah, A., 2002. "Conflict between Work and Family Roles of Employed Women in Malaysia". In: Proceedings of the 17th Annual Conference of the Society for Industrial and Organisational Psychology, Toronto, Ontario, Canada.
15. Walton, R.E "Quality of working life: what is it?" Sloon Management Review, fall1973, pp 11, 21.

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Viral Marketing – An Overview

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Abstract

What is viral marketing and why is it important for marketers today to understand and utilize? This paper addresses how marketing has become viral due to technological advances and growth of social media sites on the Internet. As the use of the Internet expands exponentially, viral marketing has begun to replace what was traditionally referred to as word-of mouth advertising. Specifically, this paper summarizes the brief history of viral marketing, examines a few successful and unsuccessful viral marketing cases and reflects on the advantages and disadvantages of this form of advertising. Furthermore, the ethical considerations that accompany viral marketing tactics are addressed as well as the implications for marketers who create viral marketing campaigns in the future.

Keywords: Viral Marketing, Word of Mouth Communication, Internet based Word of Mouth Communication.

Introduction

Marketers have been using electronic tools for many years, but the Internet and other new technologies created a flood of interesting and innovative ways to provide and enhance customer value. Not only did this challenge the fundamental basics of traditional marketing, but it also helped to shape the practice of modern marketing. Viral marketing is an advertisement that is in some way tied to an e-mail. It can be attached to the e-mail or placed in the body of the e-mail. "Viral Marketing" is a technique whereby information related to products, services or companies are "seeded" strategically. Viral marketing is a form of advocacy or word-of-mouth endorsement marketing. One customer passes along the message to other potential buyers. The name "viral" is derived from the image of a person being infected with the marketing message, then spreading it to friends like a virus. The major difference, however, is that the customer voluntarily sends the message to others. It does not occur automatically; the paper first reveals the origins of viral marketing, followed by the

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six principles that create an effective viral marketing campaign. Next, the paper consists of the examples of companies that have succeeded and some that have failed in implementing viral marketing campaigns and expands upon the characteristics that are common in successful campaigns. At the end, the paper concludes with the future trends and lifeline of viral marketing.

The Origin of Viral Marketing

Initially, the term viral marketing was developed by Juvertson and Draper (1997) which used to describe free e-mail service that was provided by Hotmail. Welker (2002), saw an analogy between viral marketing and living biological virus. Knight (1999) suggests that viral marketing is similar to "digitalized sneeze", one characterized by the release of "millions of tiny particles that can infect others who come into contact with them". Wilson (2000) defines it as "any strategy that encourages individuals to pass on marketing message to others, creating the potential for exponential growth in message's exposure and influence. Like viruses, such strategies take advantage of rapid multiplication to explode the message to thousands, to millions". Viral marketing has become an increasingly popular promotional tool (Kirsner 2005). The research of Ferguson (2008) indicates that through the "proliferation of broadband access and its attendant social networks, video-sharing sites and blogs, word-of-mouth now spreads at the speed of thought".

Shukla (2010) claims that the term viral marketing is coined by the Harvard Business School professor Rayport (1996). Among the first to write about the technique of viral marketing is media critic Douglas Rushkoff in his 1994 book *Media Virus: Hidden Agenda in Popular Culture*. Rushkoff (1994) creates the term and concept of media virus or viral media and describes that media like viruses is mobile, easily duplicated and spread as non-threatening. As to the technique of viral media, a message or image is presented to a susceptible audience in a way that it will essentially affect the recipient like a virus and the infected person will pass the message to others effectively like a virus (Rushkoff, 1996)

Source: i-DoThink.com

Viral is further marketing popularized as network-enhanced word-of-mouth advertising by the venture capitalist Steve Jurvetson and Tim Draper (Jurvetson, 1997) who describe Hotmail's e-mail practice of attaching its own advertisements with outgoing mail from its users (Palka, Pousttchi & Wiedemann, 2009; Rayport & Jaworski, 2004; Shukla, 2010; Swanepoel et al., 2009). Hotmail has become one of the first to exploit online viral marketing since its e-mail service was launched in the late 1990s, when every outgoing e-mail contained a short message at the bottom with a link for people to click and sign up. In 1996, Steve and Tim also took advantage of viral marketing as a new phenomenon to promote the adoption of Hotmail, a free web-based e-mail service provider, and viral marketing launched this e-mail system from zero to 12 million subscribers in only18 months at very little cost (Shukla, 2010).

1. **Word of Mouth Communication** Cruz and Fill (2008) identify word of mouth as person to person communication among consumers concerning their personal experience with a product or firm.
2. **Internet – based word of mouth marketing.** The advent of the Internet has brought new opportunities for both marketers and consumers to spread or receive messages about a product or service and has provided the new platform for the traditional word of communication (Datta et al, 2005)

Viral Marketing Concept

Viral marketing is successful because there are so many customers who are willing to pass along just about any message, as long as it is valuable or beneficial. Most people, who receive valuable viral messages, pass

them on to other interested people. Word-of-mouth communication increases sales, brand awareness, and market coverage. Word-of-mouth marketing provides you with benefits that you cannot get from any other form of online advertising. Through viral e-mail marketing you get the best way to

i. Reach the most targeted audience
ii. Increase sales and improve online awareness by many folds
iii. Cost-effectively build brand recognition and interest in your offerings

Key Principles of Viral Marketing

Marketers attempting a viral marketing campaign must measure the effort of the campaign by setting targets for it and taking solid baseline reports before starting it. Rasmusson (2000:18) stresses the importance of making sure that any viral marketing campaign is integrated with other marketing efforts. According to Wilson (2000:2), an effective viral marketing strategy comprises six characteristics, namely:

1. It gives away products or services for free.
2. It provides for effortless transfer to others.
3. It scales easily from small to very large.
4. It exploits common motivations and behaviours.
5. It uses existing communication networks.
6. It takes advantage of other resources to get the word out.

Promotional Techniques

Viral marketing is a simple but powerful tool for promoting your products and resources to a wide majority of the audience. For successfully promoting your resources through viral advertising it is possible to make use of the existing social networks and other available resources. Through the information provided on these social networks, you are able to sort out your advertising requirements. The other viral advertising campaign tools and procedures that can be used to construct an effective promotion strategy for your online business include the following:

a) Building easily, transferable and simple promotion messages
b) Presenting affiliate programs
c) Designing free e-books
d) Offering free services and products
e) Providing video clippings and images
f) Offering suitable rewards for the referrals
g) Developing effective and interesting blogs
h) Submitting interesting articles
i) Granting access to online contests and games
j) Offering free software downloads
k) Providing newsletters and fora

Successful Viral Campaigns

1. Hotmail and Indian pang league are classic examples of adopting viral marketing strategy.
2. Monster.com and Naukri.com are also the beneficiaries of this form of marketing.
3. Amway, Hindustan Lever and Tupperware have also implemented such marketing concept.
4. Angry Birds Space Video campaign was one of the most viewed viral videos.
5. Vodafone Zoo Zoo ads which were series of 30 ads have also added to the success list of Viral Marketing. After launching the campaign, Vodafone's subscription rates increased.
6. P&G's "Thank You Mom" global campaign was released in April, 2012 to hype the Olympics. The ad went viral, amassing over 2 million viewers on YouTube shortly after its release. It was successful because of its sincerity, timeliness and universal appeal.
7. It's not just the hard core industries who are its beneficiaries but entertainment industry is also in the list. The song named Kolaveri Di & Gangnam Style is a perfect case of viral marketing, which had created a huge difference in the world of publicity.
8. Films like Jaane Tu Ya Jaane Na, Ra-One, 3 idiots, Zindagi Na Milegi Dobara and many more have added to their income with help of their viral campaigns.

Unsuccessful Viral Campaigns

SONY Company Entertainment in 2006 tried to increase the sale of their PSP video game system by hiring a marketing agency to start a fake blog called

alliwantforxmasisapsp.com. The blog staged two guys trying to convince their friends and family on getting them PSP for Christmas. However, viewers caught on to the scheme and Sony took a negative backlash from the press and public for trying to trick their consumers with a fake market haven. Viral campaign ended soon with Sony pulling the blog altogether and posting an apology to everyone. The reason for failure was that Sony had failed to realize that consumers are smart and can figure out if message is authentic or not.

General Motors decided to have a contest on promoting their new Tahoe truck by having internet user create their own digital commercials for them. Entrants of contest could choose from range of clips and sound tracks provided on webpage and write their own text to create their own advertisement. The idea was to have the users generate buzz by sharing their own creations on channels such as YouTube. The campaign was successful in this aspect, but it was not what GM had hoped for. The user-generated advertisements that received the most buzz and views were the ones that slandered the brand and its gas guzzling truck, with many of contents being "offensive and inflammatory".

In May 2009, in case of KFC, Oprah Winfrey offered her viewers a free coupon for KFC's new grilled chicken. The promotion was successful & Oprah's KFC coupons were fifth most popular searched items on Google. The demand was too overwhelming to handle due to insufficient inventory. Then KFC CEO apologized to customers and gave discounts on future purchases. Mc Donald's created "I'd hit it" campaign to target youth in US. They created a banner ad and put in ESPN.COM website in 2007. They incorporated youth slang in it to go viral. They didn't understand correct meaning and context of usage. The meaning of phrase was "I would love to have sex with her". They failed to attract customers miserably. Many companies like General Motors, Nokia, and Starbucks have also added to the list of viral flops making the list endless.

Conclusion

The future of viral marketing is bright. As a rather modern form of advertising, the opportunities that surround the use of viral marketing are boundless. What originally began as a simple tag line at the bottom of e-mail messages developed into a worldwide marketing phenomenon utilized by all the top brands around the globe. Similar to various other marketing campaigns, viral marketing can be designed effectively as well as ineffectively. Therefore, six universal principles were established as a guide to create successful viral marketing campaigns. Viral marketing is a powerful way to reach the customers as a marketing strategy, and when applied correctly, can boost sales for the right product and speed up the transition from the stage of early adoption to widespread use. In spite of various memorable unsuccessful campaigns, the best part is that it doesn't require a product with a wow factor in order to raise awareness and generate buzz. Viral campaigns, whether ultimately liked or disliked, are often welcomed by the receivers and with a successful technique, merged with loyalty marketing efforts, marketers can identify proper scenario and build support with high end segment.

Reference

1. Viral Marketing from www.wikipedia.com
2. The six principles viral marketing by Dr.Rolph F.Wilision,E-commerce "web marketing" Feb 1,2005
3. International Journal of Marketing,Financial services & Managemant Research, Viral marketing through social marketing, Vol 1 issue 7 july 2012
4. Critical factors of viral marketing campaigns 1 Ed vol 3, International Journal of Business Science and applied management 2008 , - Online
5. Ferguson (2008) WOM and viral marketing-Taking the temparture of hottest trends in marketing, Journal of Consumer marketing 25(3) 179 -182,
6. On-line – www.Indian research journal.com
7. H.B.Klopper , viral marketing a powerful but dangerous marketing tool, South African journal of Information management Vol 4(2) June 2002
8. IJMHRM, The study of E-commerce service system in Global Viral Marketing strategy vol (3) issue 1,2012.

Section 2

SCIENCE

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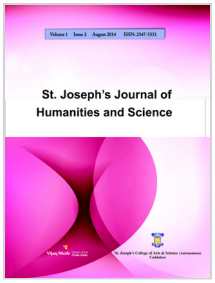

Study of Biochemical Analysis and Antibacterial Activity of *Glycyrrhiza Glabra* Root Extracts

- Dr. K. Prabu*
- P. Kanagalakshmi**

Abstract

Phytochemical analysis, biochemical analysis, *in vitro* antioxidant activity, *in vitro anti* inflammatory activity, *in vitro* antiarthritic activity and antibacterial activity of root extracts of *Glycyrrhiza glabra* were studied. The aqueous and ethanolic root extracts were tested for the presence of phytochemicals. The anti-inflammatory activity of *Glycyrrhiza glabra* at 250, 500,750,1000 mcg/ml were studied using human red blood cell membrane (HRBC) stabilization method. The anti-arthritic activity of *Glycyrrhiza glabra* at the same concentration was analysed using bovine serum albumin denaturation (BSA) method. Diclofenac, at concentration of 1000 mcg/ml, was assessed as standard anti-inflammatory and anti-arthritic drug. Antibacterial activity was evaluated using Agar well diffusion method. Phytochemical screening revealed the presence of alkaloids, flavonoids, glycosides, saponins, tannins, and terpenoids. The extracts of *Glycyrrhiza glabra* had shown significant amount of ascorbic acid and catalase. The aqueous and ethanolic extracts of *Glycyrrhiza glabra* results showed significant protection of HRBC and significant inhibition in BSA denaturation and which are comparable to standard drugs diclofenac. Aqueous and ethanolic extracts of *Glycyrrhiza glabra* exhibited significant antibacterial activity. All the analysis was made with the use of standard procedure. These results indicate the Anti-inflammatory, Antiarthritic and antibacterial potential of the *Glycyrrhiza glabra* root extracts and can be used as a promising herb in treating the clinical ailment.

Keywords: Phytochemical, Antioxidant activity, Anti-inflammatory activity, Antiarthritic activity, Anti bacterial activity, *Glycyrrhiza glabra.*

Introduction

The world is abundant with natural and medicinal plants. Medicinal plants are now more focused than ever because they have the capability of producing many benefits to society indeed to mankind, especially in the line of medicine and pharmacology. The medicinal power of these plants lies in phytochemical constituents that cause definite pharmacological actions on the human body [1]. Phytochemical, natural compound occur in plants such as medicinal plants, vegetables and fruits that work with nutrients and fibers to act against diseases or more specifically to protect against diseases.

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Glycyrrhiza glabra, family Leguminoseae, is a plant which grows in India and other countries of the world. Its roots possess some nutritive value and medicinal properties. They are widely used as a cold beverage, in preparing some pharmaceutical preparations such as haematinic pills and to disguise the bitter taste of other remedies [2]. It is a very sweet, moist, soothing herb that detoxifies and protects the liver and is also a powerful anti-inflammatory, being used in conditions as varied as arthritis and mouth ulcers. Phytochemical analysis of *Glycyrrhiza glabra* root extract showed that it contains saponin, triterpenes (glycyrrhizin, glycyrrhetinic acid and liquirtic acid), flavonoids (liquirtin, isoflavonoids and formononetin) and other constituents such as coumarins, sugars, amino acids, tannins, starch, choline, phytosterols and bitter principles[3, 4].Aim of the study was to optimize extraction methods in order to maximize the recovery of secondary metabolites in the crude extracts of *Glycyrrhiza glabra*.

In the present study, an attempt has been made to identify the active ingredients present in the root powder extracts (Different solvents) of *Glycyrrhiza glabra* plant and was subjected to phytochemicals screening, Antioxidant activity (Enzymatic and Non-enzymatic), *In-vitro* anti-inflammatory activity on human red blood cell membrane, *In-vitro* anti-arthritic activity on Inhibition of protein denaturation and Antibacterial activity by well diffusion method.

Materials And Methods

Collection of *Glycyrrhiza Glabra* Root

The plant of *Glycyrrhiza glabra* root was collected from Chetpet, in Thiruvannamalai district. The Plant was recognized based on the plant anatomy. The plant was washed thoroughly in tap water and the stem was removed from the plant. The root parts of the plant were air dried in the shade for six days. The plant samples were grounded into uniform powder using milling machine. The powder was used for the further studies.

Preparation of Extracts

Aqueous Extract

Aqueous extract of the sample was prepared by soaking 10g of dried powder in 100ml of distilled water for 24 hours. The extract was filtered using the No: 1 Whatmann filter paper and it was used for further studies.

Ethanol Extract

Ethanol extract of the sample was prepared by soaking 10 grams of dried powder in 100ml of Ethanol for 24 hours. The extract was filtered using the Whatmann No.1 filter paper and it was used for further studies.

Phytochemical Screening was carried out using standard procedures of Harborne, quantitative analysis of Glucose by ortho-Toluidine Method, Estimation of Protein by Lowry's Method, Estimation of tannins by Tyler and Herbalgram & Harborne, antioxidant analysis of Estimation of Ascorbic acid by Roe & Ruther, Determination of Catalase by Sinha method. Determination of total phenol contents by Singleton & Rossi, *In-vitro* anti-inflammatory activity of *Glycyrrhiza glabra root* (GGR) ethanol Extract on human red blood cell (HRBC) stabilization method , *In-vitro* Anti-arthritic activity of *Glycyrrhiza glabra* root (GGR) extract on Inhibition of (protein) bovine serum albumin (BSA) denaturation method, antibacterial activity by Agar well diffusion method.

Results and Discussion

The results confirm the presence of constituents which are known to exhibit medicinal as well as physiological activities. The phytochemical characteristics of the root extract of *Glycyrrhiza glabra* investigation reveal the presence of medicinally active constituents like tannins, Alkaloid, terpenoids, steroids and saponins in the leaves of *Glycyrrhiza glabra*. While Flavnois, Phlobatannins, Glycosides were absent in aqueous extract, the alkaloids contained in plants are used in medicine as anesthetic agents [15]. The presence of saponins in plants have been reported to be responsible for the tonic and stimulating activities observed in Chinese and Japanese medical herbs [16] . The results obtained in this study thus suggest that the identified phytochemical compounds may be the bioactive constituents responsible for the efficacy of the root of the plants studied. The presences of Phytochemical compounds have also been confirmed to have antimicrobial activity [17]. Hence it could be inferred that the plant extracts could be a source for the industrial manufacture of drugs useful in the chemotherapy of some microbial infection.

The qualitative phytochemical screening of *Glycyrrhiza glabra* investigated were summarized in Table - 1. The results of analysis showed that *Glycyrrhiza glabra* contains most of the phytochemical

in root extract. Ethanol and aqueous extracts of root gave similar results for alkaloids, carbohydrates, saponins and proteins. *Glycyrrhiza glabra* root extract contains alkaloids, carbohydrates, Glycosides, proteins, Saponins, Tannins, Terpenoids, Anthraquinone and Polyphenols as phytochemical constituents as shown in the present study on ethanol and aqueous solvent extracts. Preliminary Phytochemical investigations revealed the presence of alkaloids. The therapeutic properties of *Glycyrrhiza glabra* are due to alkaloids documented to possess antibacterial action.

Polyphenols possess several antioxidant mechanisms including scavenging or quenching free radicals, chelating metal ions, and inhibiting enzymatic systems responsible for free radical generation. The potent antioxidant activity of Polyphenols may provide the best protection against elevated oxidative stress. The importance of alkaloids, saponins and tannins in various antibiotics used in treating common pathogenic strains has recently been reported the antibacterial properties of tannins were also reported.

Quantitative analysis was carried out in aqueous, and Ethanolic extracts prepared from root powders of *Glycyrrhiza glabra* and the results were presented in Table – 2 & figure-1. The glucose content of *Glycyrrhiza glabra* root extract was higher in ethanol extract (250mg %) compared to aqueous extract (220mg %). Similarly the protein content of *Glycyrrhiza glabra* root extract was higher in Ethanolic extract (845mg %) compared to aqueous extract (115mg %).

The Total Phenolic content of *Glycyrrhiza glabra* extract was higher in Ethanol extract (263mg %) when compared to aqueous extract (140mg %). The Tannin content of *Glycyrrhiza glabra* leaf extract was higher in Aqueous extract (70mg %) when compared to ethanol extract (15mg %). Quantitative Results indicate that *Glycyrrhiza glabra* are rich in protein, and antioxidant components such as ascorbic acid, catalase, etc. In view of the current research focusing on exploiting plants as sources of antioxidants, potential exists for exploring the antioxidant properties in food and biologic systems. Several of the plant-derived phenolic compounds, such as flavonoids, may be successful target antioxidants to treat oxidative stress.

The results of *in-vitro* anti-inflammatory activity of *Glycyrrhiza glabra* on human red blood cell membrane were given in figure-2. *In-vitro* anti-inflammatory activity of *Glycyrrhiza glabra* was performed by using human red blood cell membrane stabilization method. *Glycyrrhiza glabra* showed significant anti-inflammatory activity in a concentration dependent manner. *Glycyrrhiza glabra* at concentration of 250 and 500 mcg/ml showed 15%, 40% 60% and 75% protection of HRBC in hypotonic solution respectably. All the results were compared with standard diclofenac at 1000 mcg/ml which showed 65% protection of HRBC in hypotonic solution respectably.

The results of *in-vitro* Antiarthritic activity of *Glycyrrhiza glabra* on Inhibition of protein denaturation method were presented in figure-3. *In-vitro* anti-arthritic activity of *Glycyrrhiza glabra* was performed by using Inhibition of protein denaturation method. *Glycyrrhiza glabra* showed significant anti-arthritic activity in a concentration dependent manner. *Glycyrrhiza glabra* at concentration of 250, 500, 750, 1000 mcg/ml showed 20%, 40%, 60%, 80% inhibition of protein denaturation respectively. All the results were compared with standard Diclofenac at 1000 mcg/ml which showed 72 % inhibition of protein denaturation respectably. Antibacterial activity of Aqueous, Ethanolic root extracts of *Glycyrrhiza glabra* against (Microorganism) Bacteria of *Escherichia coli, Klebsiella pnemoniae, Proteus vulgaricus, Proteus mirabilis, Pseudomonas, Staphylococcus aureus, Salmonella typhi* and the results shown in figure 4.

Table 1: Phytochemical Screening Of Aqueous And Ethanolic Extract Of *Glycyrrhiza Glabra*

S. No	Test / Root Extract	Aqueous	Ethanol
1.	**Test for Alkaloids**		
	a) Mayer's test	+	+
	b) Wagner's test	+	+
	c) Dragendorff's test	+	+
2.	**Test for flavonoids**		
	a) Shinoda's test	+	+
	b) Alkaline reagent test	+	+
3.	**Test for carbohydrates**		
	a) Benedict's test	+	+
	b) Molisch's test	+	+
4.	**Test for glycosides**		
	a) Borntrager's test	+	+
	b) Keller – Killani test	-	+
5.	**Test for Proteins**	+	+
	b) Biuret test	+	+
6	**Test for saponins**		
	a) Froth test	+	+
	b) Lead acetate test	+	+

7	**Test for Tannins**		
	a) Ferric chloride test	+	+
	b) Lead acetate test	+	+
8	**Test for Terpenoids**		
	a) Salkowski test	+	+
9	**Test for Anthraquinones**		
	a) Ammonia test	+	+

- → indicates the absence of phytochemicals,
+ → indicates the presence of phytochemicals.

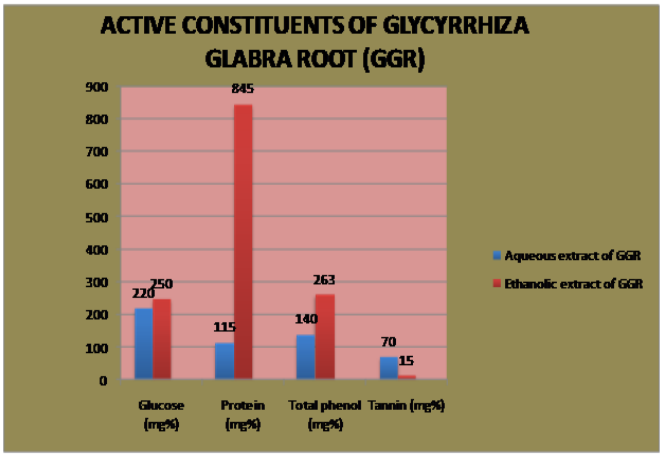

Figure 1: Active Constituents of Glycyrrhiza Glabra Root

Table 2: Non- Enzymatic-Antioxidant and Enzymatic-Antioxidant components of Glycyrrhiza glabra

S.No	Antioxidant Components	Aqueous extract (Mg %)	Ethanol extract (Mg %)
1	Vitamin C	12.5	20.8
2	Catalase	480	640

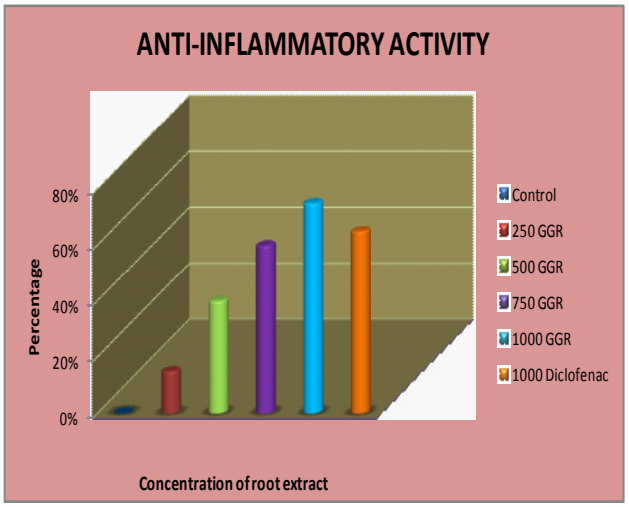

Figure 2: Anti Inflammatory Activity

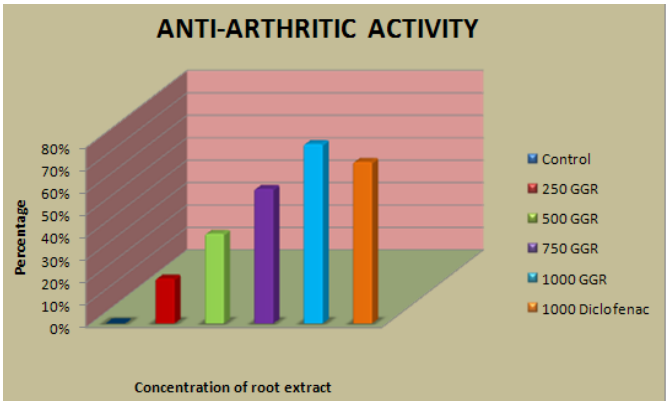

Figure 3: Anti-Arthritic Activity

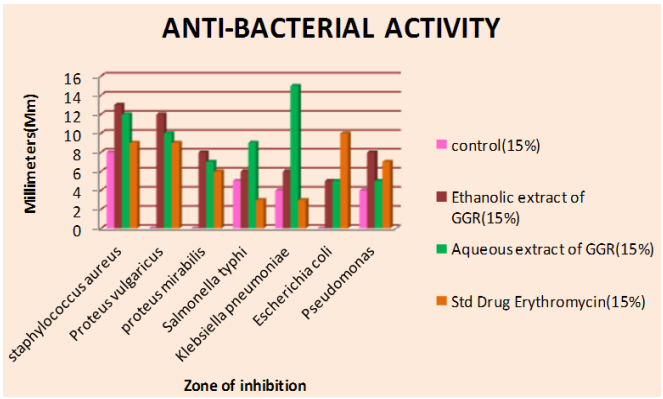

Figure 4: Anti-bacterial activity

References

1. Akinmoladun AC, Ibukun EO, Afor E, Obuotor EM, Farombi EO (2007). Pytochemical constituents and antioxidant activity of extract from the leaves of the Ocimum graticcimum. *Sci. Res. Essay*, 2: 163-166.
2. Fenwick, G.; Lutomski, J. and Nieman, C. (1990): Glycyrrhiza glabra L. (Liquorice): Composition, uses and analysis. *Food Chem.,* 38(2): 119- 143.
3. Fukai, T.; Baosheng, C.; Maruno, K.; Migakawa, Y.; Konoshi, M.; Nomura, T. and Cai, B. (1998): An isopernylated flavonone from Glycyrrhiza glabra and re-assay of liquorice phenols. *Phytochem.,* 49: 2005-2013.
4. Arystanova,T.; Irismetov, M. and Sophekova, A.(2001): Chromatographic determination of glycyrrhizinic acid in Glycyrrhiza glabra preparation. *Chem. Nat. Com.,* 37: 89-91.
5. Harborne JB (1973). *Phytochemical methods,* London Chapman and Hall, Ltd, pp. 49-88.

6. Lowry, O.H., Rosenbrough, N.J., Farr, A.L., Randal, R.J., 1951. Protein measurement with Folin-phenol reagent. *Journal of Biological Chemistry.,* 193, 265–275.
7. Tyler V (1994). *Phytomedicine in Western Europe*: their potential impact on herbal medicine in the United States Herbalgram; 30:24-30.
8. Roe, J.H., and Kuether, C.A., The determination of ascorbic acid in whole blood and urine through the 2,4-dinitrophenylhydrazine derivative of dehydro-ascorbic acid. *J. Biol. Chem.,* 1943, 147,399.
9. Artenie, V., Ungureanu, E., Negur, A. M., (2008): Metode de investigate metabolismuluiglucidici lipidic–manualdelucrripractice.*EdituraPim.,*182p.
10. Singleton, V. L., & Rossi, J. A. (1965). Colorimetry of total phenolics with phosphomolybdic-phosphotungstic acid reagents. *American Journal of Enology and Viticulture*, 16, 144–153.
11. AzeemAK, Dilip C, Prasanth SS, Junise V, Hanan Shahima. Anti-inflammatory activity of the glandular extracts of Thunnus alalunga. *Asia Pac J For Med*., 2010; 3(10): 412-420.
12. Deshpande V, Jadhav VM and Kadam VJ. In-vitro antiarthritic activity of Abutilon indicum (Linn.) Sweet. *Journal of Pharm. Res.,* 2009; 2(4): 644-645.
13. Murray PR, Baron EJ, Pfaller MA, Tenover FC, Yolken HR Manual of Clinical Microbiology, 6th Ed. ASM Press, *Washington DC,* 1995; 15-18.
14. Ismaila Y. Sudi, Denban M. Ksgbiya1 and Emmanuel K. Muluh1, Nutritional and phytochemical screening of Senna obtusifolia indigenous to Mubi nigeria, *Advances in Applied Science Research.,* 2(3), 432-437 (2011).
15. Mukeshwar Pandey, Mousumi Debnath and Etal, Phytomedicine: An ancient approach turning into future potential source of therapeutics, *Journal of Pharmacognosy and phytotherapy.,* 3(1), 113-117 (2011).
16. Victor Njoku O. and Chidi Obi, Phytochemical constituents of some selected medicinal plants, *African Journal of Pure and Applied Chemistry.*, 3(11), 228-233 (2009).
17. Alagesaboopathi C. and Sivakumar R., Antimicrobial properties of various extracts of andrographis neesiana wight-an endemic medicinal species from india, *International Journal of pharmatech research*, 3(1), 27-31 (2011).

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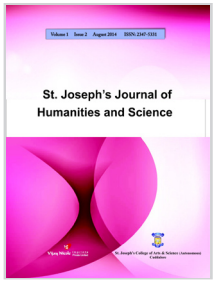

Production of Siderophore Using Bacterial Isolates From Rhizosphere of Paddy

- P. Poonguzhali*
- M. Saranya**

Abstract

The Siderophore productions of the bacterial isolates were investigated in the present study which is obtained from the rhizosphere of paddy. Among the total of thirty six isolates examined for the siderophore production using CAS (Chrome azurol sulfonate) agar plate assay, ten were producing siderophore activity. The positive bacterial isolates were belonging to the species of *Bacillus* species, *Pseudomonas* species, *Staphylococcus* species and *E. coli*. The obtained positive isolates were further subjected to the production in the succinate medium with 1% inoculum. Among the various isolates, *Pseudomonas* species were found to exhibit high siderophore production of 92% and 83% respectively.

The best Siderophore producer was selected and processed with the optimization process. The parameters such as the pH, concentration of two different carbon sources (sucrose and succinic acid) along with the incubation time were examined for the optimization of siderophore. The highest siderophore production was observed at neutral pH. While with the sucrose and succinic acid as the carbon source, the high production was obtained to be the same with concentration of 1.5% whereas the effect of incubation period over the carbon sources revealed to be much decreasing when compared with maximal production. Thus, the potent organism from the rhizosphere region of paddy having the high siderophore activity could be subjected to industrial production for various applications.

Keywords: Siderophore, Chrome azurol sulfonate, Rhizosphere.

Introduction

Siderophores are defined as relatively low molecular weight ferric iron specific chelating agents synthesized by micro-organisms growing under low ionic stress. Chemically siderophores is an iron binding proteins ranging from 400-1500 Daltons in its molecular weight. They are produced by a wide range of micro-organisms under iron limiting conditions. Siderophore serve as the iron specific extracellular ligand to aid in the solubilisation and assimilation of iron. Microbial siderophore may stimulate plant growth directly by increasing the availability of iron in the soil surrounding the roots or indirectly by competitively inhibiting the growth of plant pathogens with less efficient iron uptake system.

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Siderophore is used in medicine for iron and aluminium overload therapy, antibiotic for better targeting and suppurative therapy (Nagoba and Vedpathak, 2011). Siderophores have potential ability to resolve various environmental problems like heavy metal accumulation, rust removal, biofouling, dye degradation, sewage treatment and bioleaching etc. Siderophores are used in rust removal, because rust consists predominantly of Fe_2O_3 molecule with trivalent iron. Growth and any factors influencing either the growth or siderophore production by Plant growth promoting rizhobacteria (PGPR) would greatly influence the efficacy of that PGPR in plant growth promotion and disease suppression. The present study deals with the determination of the siderophore production by the bacterial isolates obtained from the rhizosphere region of the paddy field.

Materials and Methods

Isolation

Soil samples were collected from the rhizosphere soil of paddy field in a sterile container and further processed aseptically to obtain the bacterial isolates on nutrient agar using spread plate technique.

Screening for Siderophore Activity

The isolates were then screened for siderophore activity by plate assay. On the sterile modified Chrome azurol sulfonate (CAS) agar plate, wells were cut and 10µl broth cultures were added in each well of different isolates. Then the plates were incubated at 37°C for 24-48 hours. After incubation, colour change from blue to yellow orange halo around the growth was noted and the size of the holes around the growth was measured, which would indicate the total siderophore activity. The purified isolates were further subjected to the biochemical characterization for identification of organisms up to the genus level. The positive isolates were identified by staining, motility and biochemical test according to Bergey's manual of Systemic Bacteriology.

Quantitative Estimation

The estimation of siderophore was quantitatively done on succinate medium for the positive isolates using 1% inoculum. The flasks were then incubated for 24-48 hours at 28°C with constant shaking at 120 rpm on rotator shaker incubator. After incubation the fermented broth was centrifuged at 10,000rpm for 15 min. Supernatant was mixed with CAS solution. After 20 minutes of incubation. The absorbance of coloured solution was measured using spectrophotometer at 630nm. Similarly the assay was also carried with reference containing 0.5ml uninoculated succinate medium and 0.5ml CAS solution. The percentage of siderophore units was estimated as the proportion of CAS colour shifted (Meyer and Abdallah, 1978) using the formula,

$$\text{Siderophore units} = (Ar\text{-}As/Ar) \times 100$$

Where,

Ar = Absorbance of reference at 630 nm

As = Absorbance of sample at 630 nm

Effect of Different Parameters

The best producer was selected among all the positive isolates and subjected to optimization. Siderophore production was determined using various parameters which include pH levels (5, 6, 7, 8 & 9), Carbon source (ranging from 0.5%, 1%, 1.5%, 2% and 2.5%) succinic acid and sucrose and Incubation period (24 hrs & 48 hrs) respectively.

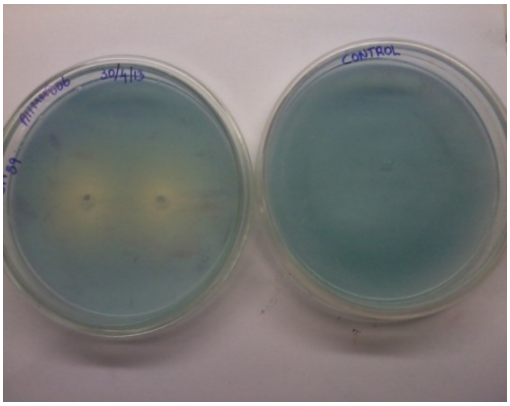
Result and Discussion

Siderophore production by bacteria is considered as important component of bacterial machinery for iron sufficiency and likely to be more important for the survival and growth in the competitive soil environment, which is usually deficient in soluble iron. The present study deals with the analysis of siderophore production by the siderophore producing bacterial isolate obtained from rhizosphere of paddy. Similarly, the earlier study of Misko and Germida (2002) suggest that the rhizosphere bacteria had an important role in the positively affects for the plant growth via different mechanisms.

Among the thirty six isolates obtained from ten samples, ten isolates (SPP50, SPP52, SPP53, SPP55 & SPP58- *Bacillus*; SPP51 & SPP61- *Pseudomonas*; SPP57- *Staphylococcus*; SPP63 & SPP69- *E. coli*) were found to produce siderophore activity, which was screened using siderophore plate assay. Isolates were screened on the CAS agar plates as described

by Schwyan and Neilands, (1987). The suggestion of modified CAS agar was made by Vagrali, (2009) and this modified CAS agar medium was employed in the present study producing yellowish orange haloes. It was indicating an iron chelator removing the iron from the blue CAS complex causing the colour change. In the earlier studies, the variation in colour changes in the CAS agar plate (yellow or orange, purple or purplish red) was observed in the production of siderophores of a differing nature by the variety of microorganisms.

Figure: 1 Screening for Siderophore by Plate Assay (Isolate SPP69)

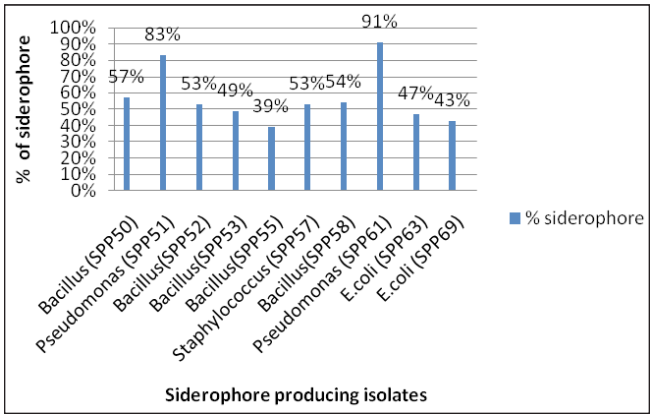


A B

Where, A is the CAS agar plate showing yellowishzone indicating the siderophore activity of the isolate SPP69 (*E.coli*) and B is the control plate.

Pal and Gokarn (2010) reported the siderophore activity exhibited by *Acinetobacter* and *E.coli* while *Bacillus subtilis* was reported by Hu and Xu, (2011). Most of the studies reported the *Pseudomonas* species from rhizosphere region (PGPR) in producing siderophore activity [Dhanya and Potty, (2007); Rachid and Ahmed, (2005)]. Similarly in our study, the ten positive isolates having the siderophore activity from rhizosphere region were identified as *Bacillus* species, *Pseudomonas* species, *Staphylococcus aureus* and *E.coli*. Five *Bacillus* species, two *Pseudomonas species*, two *E.coli* isolates and a *Staphylococcus* species were determined. In the quantitative estimation maximum percentage of siderophore production were obtained from two of the isolates which were belonging to the *Pseudomonas* species of about 91% and 83% respectively. Similar findings was also been reported by Sayyed and Chincholkar, (2010). Under iron deficiency conditions, microorganisms produce siderophores for Fe acquisition. Hence siderophores may serve as iron sources or as iron competitors for organisms, depending on the ability of the organisms to acquire iron from the stable iron siderophore complex.

Figure: 2 Percentage of Siderophore Production of Bacterial Isolates



Optimization of liquid culture conditions such as nutrients and other conditions such as pH and incubation period has profound impact on the quality and quantity of siderophore production. Correlating with the earlier reports of Hu and Xu,(2011) with increasing pH, siderophore production decreases that alkaline pH helps in excess solubilisation of iron, which increases their own content of the medium and results in decrease of siderophore production. Effect of the pH play a vital role in the siderophore production by the isolates, which was been clearly indicated from the data obtained. Moreover, the maximum siderophore production was detected to be high with the carbon source sucrose 83% when compared with the carbon source succinate. While the siderophore production using *Pseudomonas fluorescens* employed by Sayyed *et al.*, (2010) insisted on the sucrose and Mannitol as carbon source. The incubation time with combined carbon sources had its significant effect over the siderophore production, which showed much decrease on prolonged incubation than 24 hours. Thus it was suggested that siderophore production is substrate dependent and crucial factors such as substrate especially the carbon source and conditions like pH and time duration has an influence over improved siderophore production.

There is an enormous scope and multi sector application of microbial siderophores, agricultural and environmental sector for the sustainability of humans, animals and plants. But the siderophore research is not initiated in most of the microbiology research laboratories. So there is a need to insist on the organism

having elevated production, which may be helpful in the bioprocess technology for the industrial production of microbial siderophores.

References

1. Dhanya M.K and Potty V.P. 2007. Siderophore production by *Pseudomonas fluorescens* isolated from the rhizosphere of *Solenostemon rotundifolius*. *J. Root Crops. 32* (2):138-140.
2. Hu Q.P and Xu J.G. 2011. A simple double layered chrome azurol S agar plate assay to optimize the production of sidorophores by a potential biocontrol agent *Bacillus*. *African J. Microbio. Res*. 5(25): 4321-4327.
3. Meyer J.M. and Abdallah M.A.1978. The florescent pigment of *Pseudomonas flurorescence* biosynthesis, purification and physical chemical properties. *J.Gen. Microbiol*. 107:319-328.
4. Misko A.L and Germida J.J. 2002. Taxonomic and functional diversity of *Pseudomonads* isolated from the roots of field grown canola. *FEMS Microb*. 42:399-407.
5. Nagoba B and Vedpathak D. 2011. Medical applications of siderophores. *Eur. J.Gen.Med*. 8(3):229-235.
6. Pal R.B. and Gokarn.K.2010. Siderophores and pathogenecity of Microorganisms. *J.Biosci Tech*. 1(3):127-134.
7. Rachid D and Ahmed B. 2005. Effect of iron and growth inhibitors on siderophores production by *Pseudomonas fluorescens*. *African Journal of Biotech*. 4(7):697-702.
8. Sayyed R.Z and Chincholkar S.B. 2010. Growth and Siderophore production in *Alcaligenes faecalis* is regulated by metal irons. *Indian Journal of Microbial.* 50(2):179-182.
9. Sayyed R.Z., Gangurde N.S., Patel P.R, Joshi S.A and Chincholkar S.B. 2010. Siderophores production by *Alcaligenes faecalis* and *Arachis hypogaea*. *Indian Journal of Biotech*. 9:302-307.
10. Schwyn R and Neilands J.B. 1987. Universal chemical assay for detection and determination of siderophores. *Anal. Biochem*.160:47-56.
11. Vagarali M.A. 2009. Siderophore production by uropathogenic *Escherichia coli*. *India*

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NMR, UV-Visible, NLO, NBO, MEP and Vibrational Spectroscopic (IR and Raman) Analysis of O-Nitrobenzamide

- Rev. Fr. S. Xavier*
- S. Sumathi**
- K. Sivakamasundari ***

Abstract

In the present methodical study, FT-IR, FT-Raman and NMR spectra of o-nitrobenzamide are recorded and the fundamental vibrational frequencies are tabulated and assigned. The vibrational wavenumbers were computed using HF and DFT methods and are assigned with the help of potential energy distribution method. Gaussian hybrid computational calculations are carried out using HF and DFT (B3LYP and B3PW91) methods with 6-31+G (d,p) and cc-pVDZ & aug-cc-pVDZ basis sets. Moreover, ^{1}H and ^{13}C NMR spectra have been analysed and ^{1}H and ^{13}C nuclear magnetic resonance chemical shifts are calculated using the gauge independent atomic orbital (GIAO) method. A study on the electronic and optical properties (absorption wavelengths, excitation energy, dipole moment and frontier molecular orbital energies) is performed using HF and DFT methods. Stability of the molecule arising from hyper conjugative interactions, charge delocalization has been analysed using natural bond orbital (NBO) analysis. The calculated HOMO and LUMO energies (kubo gap) are displayed in the figures, which show the occurrence of charge transformation within the molecule. Besides frontier molecular orbital (FMO) energy, molecular electrostatic potential (MEP) was also calculated. NLO properties related to polarizability and hyperpolarizability are also discussed. The local reactivity of the molecule has been studied using the Fukui function.

Keywords: o-nitrobenzamide; gauge-independent atomic orbital; chemical shifts; FMO, Fukui function.

Introduction

O-nitrobenzamide is an organic compound, which consists of nitro; carbonyl and amide groups are attached to the phenyl ring. It reacts with azo and diazo compounds to generate toxic gases. Flammable gases are formed by the reaction of O-nitrobenzamide with strong reducing agents. O-nitrobenzamide has very weak bases (weaker than water). These derivatives are less basic yet and in fact react with strong bases

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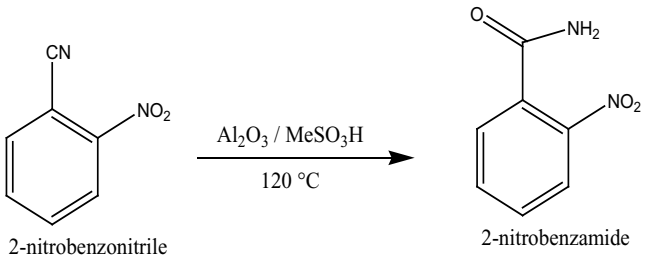
to form salts. That is, they can react as acids. Mixing amides with dehydrating agents such as P_2O_5 or $SOCl_2$ generate the corresponding nitrile. The combustion of these compounds generates mixed oxides of nitrogen (NOx). It is a stable compound and does not undergo polymerization. O-nitrobenzamide is easily oxidized by using Strong oxidizing agents. Exposure to air or moisture over prolonged periods destroys the nature of the amide.

The IUPAC name of O-nitrobenzamide is 2-Nitrobenzamide. The molecular formula of O-nitrobenzamide is $C_7H_6N_2O_3$ and the molecular weight is 166.13. It is a kind of beige crystalline powder and belongs to the classes of Aromatic Carboxylic Acids, Amides, Anilides and Carbonyl Compounds; Organic Building Blocks. Other synonyms of o-nitrobenzamide are: 2-Nitrophenylformamide;benza mide, o-nitro-;2-Carbamoylnitrobenzene.

Preparation of 2-Nitrobenzamide

It can be prepared by the reaction 2-nitro-benzonitrile with Al_2O_3 and $MeSO_3H$. The reaction time is 15 minutes at reaction temperature of 120 °C. The yield is about 90%.



2-nitrobenzonitrile 2-nitrobenzamide

Applications

2-Nitrobenzamide was used in the synthesis of novel fluorogenic chemosensors based on urea derivative of 2-(2′-aminophenyl)-4-phenylthiazole. It was also used in the synthesis of quinazoline-2,4(1*H*,3*H*)-diones, an important class of pharmaceutical intermediates[1].

There is provided 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide for various uses, as well as pharmaceutical compositions and devices comprising 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide [2]. There are also other methods provided for reducing reducible compounds (such as reduction-activated prodrugs, e.g. tretazicar) by contacting those compounds with α-hydroxycarbonyl compounds capable of forming cyclic dimers.

Experimental Details

The spectra of o-nitrobenzamide are purchased from Sigma–Aldrich Chemicals, USA. The FT-IR spectrum of the compound is recorded using a Bruker IFS 66V spectrometer in the range of 4000–500 cm^{-1}. The spectral resolution is ±2 cm^{-1}. The FT-Raman spectrum of the same compound is also recorded using the same instrument with FRA 106 Raman module equipped with Nd: YAG laser source operating at 1.064 μm line width with 200 mW power. The spectra are recorded in the range of 3500–400 cm^{-1} with a scanning speed of 30 cm^{-1} min^{-1} of spectral width 2 cm^{-1}. The frequencies of all sharp bands are accurate to ±1 cm^{-1}.

Computational Methods

In the present work, HF and some of the hybrid methods, B3LYP and B3PW91, are carried out using the basis sets 6-31+G (d,p) and cc-pVDZ & aug-cc-pVDZ. All these calculations are performed using the GAUSSIAN 09W [3] program package on an i7 processor in a personal computer. In DFT methods, B3LYP is the combination of Becke's three-parameter hybrid function, and the Lee–Yang–Parr correlation function [4, 5]. B3PW91 is the combination of Becke's three parameter exact exchange-function (B3) [6] and Perdew-Wang (PW91) correlation function [7, 8]. The optimized molecular structure of the molecule is obtained using the Gaussian 09 and Gaussview program and is shown in Fig. 1. The comparative optimized structural parameters such as bond length, bond angle and dihedral angle are presented in Table 1. The observed (FT-IR and FT-Raman) and calculated vibrational frequencies and vibrational assignments are presented in Table 3. Experimental and simulated spectra of IR and Raman are presented in Fig. 2 and 3, respectively.

Table 1: Optimized Geometrical Parameters of O-Nitrobenzamide

Geometrical Parameter	HF/6-31+G (d, p)	B3LYP/ cc-pVDZ	B3LYP/ aug-cc-pVDZ	B3PW91/ cc-pVDZ	B3PW91/ aug-cc-pVDZ
Bond length(Å)					
C1-C2	1.3824	1.3965	1.3953	1.3932	1.3926
C1-C6	1.3844	1.3935	1.3947	1.3915	1.3923
C1-H7	1.0720	1.0890	1.0873	1.0896	1.0880
C2-C3	1.3885	1.4019	1.4020	1.3988	1.3989
C2-N16	1.4608	1.4787	1.4766	1.4726	1.4707
C3-C4	1.3878	1.4020	1.4012	1.3992	1.3986
C3-C11	1.5149	1.5229	1.5171	1.5181	1.5133
C4-C5	1.3873	1.3966	1.3977	1.3946	1.3953
C4-H8	1.0747	1.0915	1.0896	1.0916	1.0901
C5-C6	1.3853	1.3987	1.3980	1.3961	1.3957
C5-H9	1.0750	1.0921	1.0901	1.0921	1.0905
C6-H10	1.0743	1.0914	1.0895	1.0914	1.0899
C11-N12	1.3538	1.3695	1.3671	1.3650	1.3633
C11-O15	1.1949	1.2165	1.2201	1.2148	1.2182
N12-H13	0.9963	1.0170	1.0123	1.0157	1.0115
N12-H14	0.9939	1.0145	1.0101	1.0133	1.0094
N16-O17	1.1921	1.2234	1.2268	1.2180	1.2213
N16-O18	1.1947	1.2273	1.2287	1.2214	1.2230
Bond angle(°)					
C2-C1-C6	119.0509	119.2607	119.1608	119.2364	119.1441
C2-C1-H7	119.5570	118.6869	119.1169	118.6622	118.9830
C6-C1-H7	121.3899	122.0522	121.7189	122.1009	121.8694
C1-C2-C3	122.3741	122.2871	122.2790	122.3120	122.3125
C1-C2-N16	117.5141	117.4046	117.5516	117.5037	117.5828
C3-C2-N16	120.0770	120.2823	120.1418	120.1508	120.0768
C2-C3-C4	117.6526	117.3564	117.5168	117.4108	117.5295
C2-C3-C11	124.1230	124.7048	124.0137	124.3306	123.9706
C4-C3-C11	117.9677	117.5738	118.1082	117.8762	118.1485
C3-C4-C5	120.8002	121.1327	120.982	121.0648	120.9504
C3-C4-H8	119.1754	118.7378	118.9565	118.7821	118.9345
C5-C4-H8	120.0145	120.1274	120.0516	120.1499	120.1057
C4-C5-C6	120.3813	120.272	120.281	120.2896	120.2985
C4-C5-H9	119.56	119.6414	119.6301	119.634	119.6228
C6-C5-H9	120.057	120.0853	120.0873	120.075	120.0772
C1-C6-C5	119.7332	119.6853	119.7707	119.6804	119.755
C1-C6-H10	119.7764	119.8309	119.7817	119.832	119.7955
C5-C6-H10	120.4902	120.4837	120.4475	120.4874	120.4493
C3-C11-N12	115.2722	114.8585	115.3178	114.6749	115.1494
C3-C11-O15	120.5307	120.5118	120.5817	120.5567	120.5548
N12-C11-O15	123.875	124.1315	123.7072	124.2923	123.8866
C11-N12-H13	115.8144	114.7257	116.3293	115.0125	116.2744
C11-N12-H14	119.3354	117.48	119.5092	117.7549	119.283
H13-N12-H14	116.7363	115.3259	117.0742	115.6925	117.0798
C2-N16-O17	117.7678	117.7686	117.8141	117.6843	117.7303
C2-N16-O18	117.0905	117.2884	117.3545	117.1495	117.2526
O17-N16-O18	125.1204	124.9316	124.8163	125.1525	125.0022
Dihedral Angle(°)					
C6-C1-C2-C3	-1.0091	-0.697	-1.1373	-0.7658	-1.1555
C6-C1-C2-N16	176.8431	177.4508	176.9525	177.1293	176.9215
H7-C1-C2-C3	179.5178	179.464	179.5239	179.4799	179.5107
H7-C1-C2-N16	-2.63	-2.3882	-2.3863	-2.6251	-2.4122
C2-C1-C6-C5	0.3858	0.3084	0.4541	0.2925	0.4699
C2-C1-C6-H10	-179.5073	-179.5693	-179.4038	-179.541	-179.3868
H7-C1-C6-C5	179.849	-179.8582	179.7749	-179.9619	179.7837
H7-C1-C6-H10	-0.0442	0.2641	-0.083	0.2046	-0.0731
C1-C2-C3-C4	0.936	0.3534	0.9839	0.5015	0.9811
C1-C2-C3-C11	-173.1128	-172.522	-171.9698	-172.2309	-172.0716
N16-C2-C3-C4	-176.8628	-177.7424	-177.0577	-177.3393	-177.0493

N16-C2-C3-C11	9.0885	9.3822	9.9886	9.9283	9.898
C1-C2-N16-O17	25.5148	16.9002	22.4557	18.5233	21.9369
C1-C2-N16-O18	-152.8936	-161.9383	-156.197	-160.1976	-156.729
C3-C2-N16-O17	-156.5814	-164.913	-159.4117	-163.534	-159.9411
C3-C2-N16-O18	25.0102	16.2485	21.9355	17.7451	21.393
C2-C3-C4-C5	-0.2555	0.3737	-0.1662	0.2273	-0.1396
C2-C3-C4-H8	-179.1085	-179.0928	-179.017	-179.13	-179.0241
C11-C3-C4-C5	174.1676	173.7685	173.2141	173.4402	173.3278
C11-C3-C4-H8	-4.6854	-5.6981	-5.6367	-5.917	-5.5566
C2-C3-C11-N12	-111.2264	-101.7148	-111.742	-105.3585	-111.4727
C2-C3-C11-O15	75.0428	86.0545	75.1947	82.226	75.5901
C4-C3-C11-N12	74.7422	85.4239	75.3431	81.9403	75.5146
C4-C3-C11-O15	-98.9886	-86.8067	-97.7202	-90.4753	-97.4226
C3-C4-C5-C6	-0.3305	-0.7522	-0.4788	-0.6837	-0.5075
C3-C4-C5-H9	-179.8526	179.6711	179.9806	179.7412	179.9487
H8-C4-C5-C6	178.5129	178.707	178.3595	178.6648	178.3639
H8-C4-C5-H9	-1.0092	-0.8697	-1.1811	-0.9102	-1.1799
C4-C5-C6-C1	0.2655	0.3992	0.3329	0.415	0.3397
C4-C5-C6-H10	-179.8422	-179.7239	-179.8101	-179.7526	-179.8045
H9-C5-C6-C1	179.7852	179.9739	179.8713	179.9881	179.8814
H9-C5-C6-H10	-0.3225	-0.1492	-0.2717	-0.1794	-0.2628
C3-C11-N12-H13	173.1876	171.3074	174.0636	171.4957	173.7856
C3-C11-N12-H14	25.5031	30.9223	24.3394	29.67	24.5916
O15-C11-N12-H13	-13.3175	-16.781	-13.1163	-16.4116	-13.5424
O15-C11-N12-H14	-161.002	-157.1661	-162.8405	-158.2373	-162.7364

Table 2: Observed and Calculated Vibrational frequencies of O-Nitrobenzamide Using HF and DFT (B3LYP & B3PW91) at the 6-31+G(d, p) & cc-pVDZ, aug cc-pVDZ Basic Sets

S. No.	Observed Frequency(cm^{-1})		Methods					Vibrational Assignments
			HF	B3LYP		B3PW91		
	FT-IR	FT Raman	6-31 +G (d, p)	cc-pVDZ	aug-cc-pVDZ	cc-pVDZ	aug-cc-pVDZ	
1	3390 vs	-	3512	3494	3535	3496	3532	υN-H (100%)
2	3390 vs	-	3392	3372	3408	3370	3403	υN-H (100%)
3	3100 s	-	3034	3087	3094	3071	3079	υC-H (95%)
4		3090 m	3008	3062	3071	3050	3060	υC-H (97%)
5		3080m	2999	3053	3062	3040	3050	υC-H (97%)
6		3050m	2987	3041	3051	3028	3039	υC-H (100%)
7	1680 vs	-	1744	1720	1683	1724	1692	υC=O (84%)
8	1600 s	-	1639	1596	1585	1608	1595	υN=O (31%) + υC=C (36%)
9	1590 w	-	1591	1559	1551	1570	1561	υN=O (35%) + υC=C (33%)
10	1580 w	-	1672	1646	1647	1652	1646	υN=O (12%) + υC-C (43%)
11	-	1570 vw	1654	1628	1629	1615	1632	δNH_2 (74%)
12	1520 vs		1556	1532	1531	1527	1525	υC-C (14%) + δHCC (48%)
13	1470 m	-	1538	1490	1485	1483	1478	υC-C (13%) + δHCC (44%)
14	1430 w	-	1501	1423	1419	1443	1438	υN=O (77%) + δONO (10%)
15	1400 m	1400 vw	1396	1391	1391	1403	1397	υN-C (30%) + υC=C (18%) + δHNC (13%) + δNCO (12%)
16	1400 m	1400 vw	1322	1388	1383	1393	1393	υC-C (78%)
17	1320 w	-	1255	1298	1303	1287	1291	δHCC (58%)
18	1270 w	1270 vw	1194	1196	1202	1191	1194	δHCC (67%)
19	1230 vw	-	1178	1271	1275	1280	1282	υC=C (17%) + υN-C (10%) + δHCC (29%)
20	1230 vw	-	1223	1257	1261	1261	1264	υC=C (15%) + δHNC (12%) + δHCC (24%)
21	1230 vw	-	1215	1216	1211	1218	1211	υO=C (12%) + υN=C (27%) + δHNC (42%)
22	1180 vw	-	1180	1184	1184	1156	1187	υN-C (12%) + δCCC (45%)
23	1130 m	-	1133	1157	1160	1163	1164	υC=C (71%) + δHCC (12%)
24	1130 m	-	1132	1109	1107	1108	1098	τHCCN (14%) + τHCCC (66%)
25	1090 vw	-	1100	1074	1070	1073	1067	τHCCN (40%) + τHCCC (42%)
26	1000 vw	1000 vw	1003	983	979	982	977	τHCCN (27%) + τHCCC (50%)
27	970 vw	970 vw	963	952	949	962	957	υN-C (10%) + γCCC (14%) + γOCN (47%)
28	890 vw	890 vw	899	875	879	878	882	τHCCC (54%) + γOCON (30%)
29	860 m	860 vw	859	844	849	844	849	γOCON (10%) + γHCC (50%)
30	850 vw	850 vw	838	833	835	833	834	δCCC (22%) + γOCNC (33%)
31	830 vw	-	823	828	824	829	825	γOCNC (27%) + γNH_2
32	790 m	790 vw	785	778	780	780	781	τHCCC (11%) + τCCCC (25%) + γOCON (36%)

33	730 w	730 vw	728	741	739	741	740	υN-C (11%) + γCCC (29%) + γONO (18%)
34	665 w	-	661	670	668	666	665	γNCO (40%) + γCCC (11%)
35	620 vw	-	617	631	626	629	625	τHNCC (38%)
36	600 vw	-	611	620	620	618.6	619	γCCN (21%) + τHNCC (14%) + τCCCC (13%)
37	570 vw	570 vw	567	1569	1368	1530	1368	γCNO (25%) + τHNCC (30%)
38	-	470 vw	467	1327	1128	1288	1123	τHNCC (76%)
39	-	440 vw	455	1265	1094	1224	1097	τCCCC (33%) + γNCCC (23%)
40	-	430 vw	1243	1218	1078	1193	1081	υN-C (30%) + γCCC (13%)
41	-	390 vw	1071	1038	930	1008	923	γCCN (20%) + τCCCC (52%)
42	-	360 vw	971	943	851	924	847	υC=C (15%) + γCNO (11%) + γCCC (17%) + γCCN (13%)
43	-	360 vw	788	775	685	752	681	γCNO (14%) + γCCN (46%)
44	-	360 vw	516	504	440	486	439	γCCC (12%) + γNCCC (24%) + γCCCC (22%)
45	-	360 vw	469	468	406	446	399	γCCC (44%) + γCCN (13%)
46	-	360 vw	333	309	276	299	276	τCCCC (41%) + γCCCC (32%)
47	-	360 vw	255	194	208	207	213	τCCNO (63%) + τCCCN (21%)
48	-	360 vw	103	73	84.37	74.91	84	τCCNO (21%) + τCCCN (65%)

vs – very strong, s – strong, m – medium, w – weak, vw – very weak
υ-stretching, δ-in-plane bending, γ-out-of-plane bending, τ-torsional

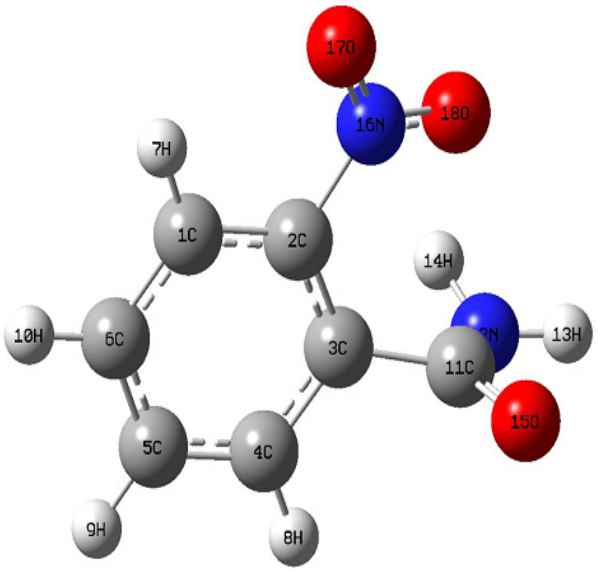


Figure 1: Molecular Structure of O-Nitrobenzamide

The ^{1}H and ^{13}C NMR isotropic shielding are calculated using the GIAO method [9] and the optimized parameters obtained from the B3LYP/cc-pVDZ method. ^{13}C isotropic magnetic shielding (IMS) of any X carbon atoms is made according to the ^{13}C IMS value of TMS, $CS_X = IMS_{TMS}-IMS_x$. The ^{1}H and ^{13}C isotropic chemical shifts of TMS (Tetramethylsilane) in gas, DMSO, methanol and ethanol are calculated using IEFPCM method with the B3LYP functional at the cc-pVDZ level. The absolute chemical shift is found between the isotropic peaks and the peaks of TMS [10]. Stability of the molecule arising from hyper conjugative interactions, charge delocalization is analyzed using natural bond orbital (NBO) analysis. The electronic properties, HOMO-LUMO energies, absorption wavelengths and oscillator strengths are calculated using the time-dependent DFT (TD-DFT) [11, 12] method with the B3LYP functional in the gas phase and the solvent phase. Moreover, dipole moment, polarizability, hyperpolarizability related to nonlinear optical (NLO) properties is also studied. The local reactivity of the molecule is studied using the Fukui function. The condensed softness indices are found and are used to predict both the reactive centers and the possible sites of nucleophilic and electrophilic attack.

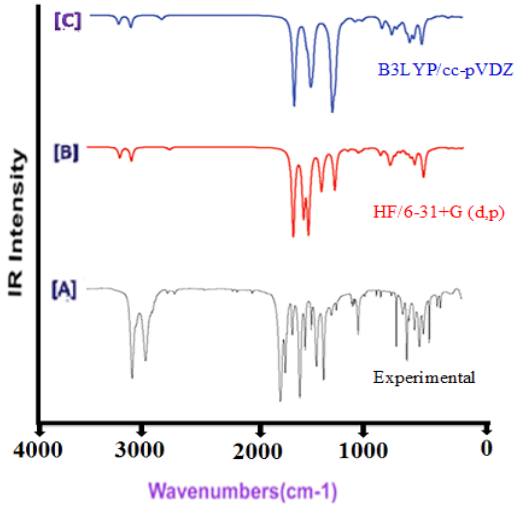


Figure 2: Experimental [A] & Calculated [B, C] FT-IR Spectra of O-Nitrobenzamide

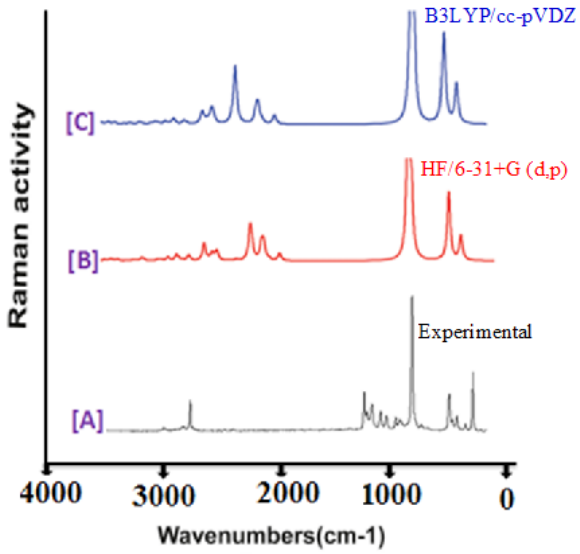


Figure 3: Experimental [A] & Calculated [B, C] FT-Raman Spectra of O-Nitrobenzamide

Results and Discussion

Molecular Geometry

From the optimized output file of Gaussian it is observed that the molecular structure of o-nitrobenzamide belongs to C_1 point group symmetry. The optimized structure of the molecule is obtained from the Gaussian 09 and Gauss view program [13] and is shown in Fig. 1. The present molecule contains one nitro group and one amide group, which are loaded in the left moiety. The hexagonal structure of the benzene is deformed at the point of substitution due to the addition of the heavy mass. It is also evident that the bond length (C1-C2 & C2-C3) at the point of substitution is 0.0054 Å, which is longer than the rest in the ring. Consequently, the property of the same also changed with respect to the ligand (nitro and amide groups). The bond angle of C1–C2–C3 is 2.0151º elevated more than C4–C5–C6 in the ring, which also confirms the deformation of the hexagonal shield. Although both C=O and NH_2 groups, the bond length values between C2–C3 and C3–C11 differed by 0.121 Å. The entire C–H bonds in the chain and the amide groups have almost equal inter-nuclear distance.

Table 3: Calculated unscaled frequencies of O-Nitrobenzamide using HF/DFT (B3LYP&B3PW91) with 6-31+(d,p) and cc-pVDZ, aug-cc-pVDZ basis sets

S. No.	Observed Frequency	Calculated frequency				
		HF	B3LYP		B3PW91	
		6-31+G (d, p)	cc-pVDZ	aug-cc-pVDZ	cc-pVDZ	aug-cc- pVDZ
1	3390 vs	3951	3661	3691	3693	3714
2	3390 vs	3816	3533	3558	3560	3578
3	3100 s	3413	3235	3230	3244	3237
4	3090 m	3384	3208	3206	3222	3217
5	3080 m	3374	3199	3197	3212	3207
6	3050 m	3360	3186	3185	3199	3195
7	1680 vs	1962	1802	1757	1821	1779
8	1600 s	1844	1672	1655	1699	1677
9	1590 w	1790	1633	1619	1659	1641
10	1580 w	1781	1618	1614	1635	1626
11	1570 vw	1761	1600	1596	1598	1612
12	1520 vs	1657	1506	1500	1511	1506
13	1470 m	1638	1465	1455	1468	1460
14	1430 w	1599	1399	1390	1428	1420
15	1400 m	1487	1367	1363	1388	1380
16	1400 m	1408	1364	1355	1379	1376
17	1320 w	1336	1276	1277	1274	1275
18	1270 w	1272	1176	1178	1179	1179
19	1230 vw	1255	1164	1162	1170	1169
20	1230 vw	1223	1151	1149	1153	1152
21	1230 vw	1215	1114	1103	1113	1104
22	1180 vw	1180	1084	1079	1057	1082
23	1130 m	1133	1060	1057	1063	1061
24	1130 m	1132	1016	1009	1013	1001
25	1090 vw	1100	984	975	981	973

26	1000 vw	1003	900	892	898	891
27	970 vw	963	872	865	880	873
28	890 vw	899	804	804	808	808
29	860 m	859	776	777	777	778
30	850 vw	846	766	764	767	764
31	830 vw	831	761	754	763	756
32	790 m	792	715	714	718	716
33	730 w	735	681	677	682	678
34	665 w	667	616	612	613	609
35	620 vw	623	580	573	579	573
36	600 vw	617	570	568	569	567
37	570 vw	572	532	519	531	520
38	470 vw	472	450	428	447	427
39	440 vw	459	429	415	425	417
40	430 vw	448	413	409	414	411
41	390 vw	386	352	353	350	351
42	360 vw	350	320	323	321	322
43	360 vw	284	263	260	261	259
44	360 vw	186	171	167	169	167
45	360 vw	169	159	154	155	152
46	360 vw	120	105	105	104	105
47	360 vw	92	66	79	72	81
48	360 vw	37	25	32	26	32

vs – very strong, s – strong, m – medium, w – weak, vw – very weak

Vibrational Assignments

In order to obtain the spectroscopic significance of o-nitrobenzamide, the computational calculations are performed using frequency analysis. The molecule has C_1 point group symmetry, consists of 18 atoms, so it has 48 normal vibrational modes. On the basis of C_1 symmetry, the 48 fundamental vibrations of the molecule can be distributed as 36 in-plane vibrations of A′ species and 12 out-of-plane vibrations of A″ species, i.e., Γ_{vib} = 36 A′ + 12 A″. In the C_1 group, the symmetry of the molecule is a non-planar structure and has 48 vibrational modes that span in the irreducible representations.

The vibrational frequencies (unscaled and scaled) calculated at HF, B3LYP and B3PW91methods with 6-311+G(d,p), cc-pVDZ and aug cc-pVDZ basic sets and observed FT-IR and FT-Raman frequencies for various modes of vibrations have been presented in Tables 2 and 3. The Frequencies calculated at the HF and B3LYP/B3PW91 methods are found to be high compared to experimental vibrations. The Inclusion of electron correlation in the density functional theory to a certain extent makes the frequency values smaller in comparison with the HF frequency data.

The calculated frequencies are scaled down to give up the rational with the observed frequencies. The scaling factors are 0.8889, 0.9390, 0.9999 and 0.9909 for HF/6-31+G (d, p). For the B3LYP/cc-pVDZ/aug-cc-pVDZ basis set, the scaling factors are 0.9544, 1.0174, 1.0919 and 1.0881/0.9578, 1.0207, 1.0976 and 1.0929. For the B3PW91/ cc-pVDZ/aug-cc-pVDZ basis set, the scaling factors are 0.9466, 1.0105, 1.0939 and 1.0871/0.9511, 1.0125, 1.0968 and 1.0921.

N−H, N=O Vibrations

In heterocyclic molecules, the N−H stretching vibrations have been measured in region 3500–3000 cm^{-1} [14]. As seen in Table 2, the two N−H stretching modes are calculated at 3494 and 3372 cm^{-1} in B3LYP. A very strong FT-IR N−H stretching vibration is observed at 3390 cm^{-1} in the experimental spectrum. Ten et al. [15] have observed these modes at 3479 and 3432 cm^{-1}, respectively, for isolated thymine. In 2-amino-4-methylbenzothiazole, V. Arjunan et al [16]. have observed the vibrational frequencies at 3417 and 3287 cm^{-1}. Cirak and Koc [17] have calculated the N–H stretching modes at 3189 and 3155 cm^{-1} for dimeric trifluorothymine. However, no Raman band is observed for the N−H stretching modes in the experimental spectra. For primary amino group the in-plane $–NH_2$ deformation vibration occur in the short range 1650–1580 cm^{-1} region of the spectrum. Therefore the very weak band observed in IR at 1570 cm^{-1} is assigned to the deformation mode of the amino group.

The most characteristic bands in the spectra of nitro compounds are due to NO_2 stretching vibrations,

which are the most useful group wavenumbers, not only because of their spectral position but also for their strong intensity [18]. The N=O stretching vibrations have been measured in region 1515-1560 cm^{-1}. A weak IR N═O stretching vibration is observed at 1430 cm^{-1}. However, no Raman band is observed for the N=O stretching modes. Hence these vibrations show good agreement with the literature values.

C–H Vibrations

The C–H stretching vibrations are normally observed in the region 3100-3000 cm^{-1} for the aromatic benzene structure, [19–20] which shows their uniqueness of the skeletal vibrations. The bands appeared at 3100, 3090, 3080, and 3050 cm^{-1} in o-nitrobenzamide are assigned to C–H ring stretching vibrations. The FT-IR bands at 1520 and 1470 cm^{-1} are assigned to C–H in-plane bending vibrations and FT-IR bands at 860 cm^{-1} are assigned to C–H out-of-plane bending vibration. V. Karunakaran et al. [21] in the molecule 4-chloro-3-nitrobenzaldehyde (CNB) have observed the bands at 3053, 3034 cm^{-1} in FT-IR and at 3079, 3052 cm^{-1} in FT-Raman spectra. The FT-IR bands at 1467, 1422 cm^{-1} and the FT-Raman bands at 1423 and 1218 cm^{-1} were assigned to C–H in-plane bending vibration of CNB. The C–H out-of-plane bending vibrations of the CNB were well identified at 989, 822 and 722 cm^{-1} in the FT-IR and 828 cm^{-1} in the FT-Raman spectra V. Arjunan et al. [22] in 4-acetyl benzonitrile, have been observed the C–H stretching peaks in IR at 3075 and 3030 cm^{-1} and in Raman spectrum at 3090, 3074 and 3025 cm^{-1}. The frequencies calculated for the present compound using B3LYP/cc-pVDZ and B3LYP/aug cc-pVDZ methods for C–H in-plane bending vibrations showed excellent agreement with the recorded spectrum as well as literature data.

C–C Vibrations

V. Arjunan et al [23] in 4-acetyl benzonitrile, have observed the C–C stretching vibrations at 1593, 1556, 1485, 1415, and 1259 cm^{-1} in IR spectrum and 1603, 1482, 1430, 1408 and 1270 cm^{-1} in Raman spectrum. The IR bands observed at 1593 and 1285 cm^{-1} were strong while the Raman band 1603 cm^{-1} was very strong. In addition, C–C–C in–plane bending vibrations have been attributed to 1002 and 844 cm^{-1} in IR spectrum and 794 cm^{-1} in Raman spectrum. The C–C–C out of plane vibrations have been observed at 337, 227 and 108 cm^{-1} in Raman spectrum. V. Karunakaran et al.[24] in the molecule 4-chloro-3-nitrobenzaldehyde have observed the C–C stretching vibrations at 1589, 1356, 1200 and 1056 cm^{-1} in FT-IR spectrum and at 1626, 1372, 1160 and 1058 cm^{-1} in Raman spectrum.

The bands due to the C–C stretching vibrations are called skeletal vibrations normally observed in the region 1430–1650 cm^{-1} for the aromatic ring compounds.[25, 26] Socrates [27] mentioned that the presence of a conjugate substituent such as C=C causes stretching of peaks around the region of 1625–1575 cm^{-1}. As predicted in the earlier references, in this title compound, the prominent peaks are found with strong and medium intensity at 1600 and 1590 cm^{-1} due to C=C stretching vibrations. The C–C stretching vibrations have appeared at 1580, 1520, 1470 and 1400 cm^{-1}. The C-C out-of-plane bending vibrations have appeared at 1130, 1090, 1000 and 970 cm^{-1}.

C—N Vibrations

The C—N vibration of the compound identification is a very difficult task, since the mixing of several bands is possible in the region. Silverstein et al. [28] assigned C—N stretching absorption in the region 1382–1266 cm^{-1} for aromatic amines. In benzamide the band observed at 1368 cm^{-1} is assigned due to C—N stretching [29]. However with the help of force field calculations, the C—N vibrations are identified and assigned in this study. A. Prabakaran et al.[30] in 7-(1,3-dioxolan-2-ylmethyl)-1,3-dimethylpurine-2,6-dione (7DDMP26D) have observed C–N, C=N stretching vibrations at 1478.19 and 1280.19 cm^{-1} in FT-IR spectrum and at 1480.00 and 1280.53 cm^{-1} in FT-Raman spectrum respectively. In our present work, C—N stretching vibrations are observed at 1400 and 1180 cm^{-1} in FT-IR spectrum. This band has been calculated at 1403 cm^{-1} by DFT method and at 1180 cm^{-1} by HF method are in very good agreement with experimental values.

C=O Vibrations

The C=O stretching frequency appears strongly in the IR spectrum in the range 1600–1850 cm^{-1} because of its large change in dipole moment. The carbonyl group vibrations give rise to characteristics bands in vibration spectra and its characteristic frequency is used to study a wide range of compounds. The intensity

of these bands can increase owing to conjugation or formation of hydrogen bonds [31]. Carthigayan et al. [32] have observed the bands at 1822 and 1842 cm^{-1} in the infrared spectrum corresponding to C=O stretching in 4,5-Bis(bromomethyl)-1,3-dioxol-2-one (45BMDO). The corresponding frequency of 4-Bromomethyl-5-methyl-1, 3-dioxol-2-one (4BMDO) was observed at 1820 cm^{-1}. A very strong IR absorption band at 1680 cm^{-1} is readily assigned to the carbonyl vibration in the o-nitrobenzamide; the corresponding DFT computed mode at 1720 cm^{-1} at B3LYP/cc-pVDZ, level is in good agreement with the observed one.

NBO Analysis

The second order perturbation NBO Fock matrix was carried out to evaluate the donor–acceptor interactions in the NBO analysis. The interaction result is a loss of occupancy from the localized NBO of the idealized Lewis structure into an empty non-Lewis orbital. For each donor (i), and acceptor (j), the stabilization energy $E^{(2)}$ associated with the delocalization i→j is estimated as

$$E^2 = \ddot{A}E_{ij} = q_i \frac{F(i,j)^2}{\varepsilon_j - \varepsilon_i}$$

Natural bond orbital analysis provides an efficient method for studying intra and intermolecular bonding and interaction among bonds, and also provides a convenient basis for investigating charge transfer or conjugative interaction in molecular systems [33]. Some electron donor orbital, acceptor orbital and the interacting stabilization energy resulted from the second-order perturbation theory [34] are where q_i is the donor orbital occupancy, are ε_i and ε_j diagonal elements and F (i, j) is the off diagonal NBO Fock matrix element reported [35, 36]. The larger the $E^{(2)}$ value, the more intensive is the interaction between electron donors and electron acceptors, i.e. the more donating tendency from electron donors to electron acceptors the greater the extent of conjugation of the whole system [37]. Delocalization of electron density between occupied Lewis-type (bond or lone pair) NBO orbitals and formally unoccupied (anti-bond or Rydgberg) non- Lewis NBO orbitals correspond to a stabilizing donor–acceptor interaction. NBO analysis has been performed on the o-nitrobenzamide molecule in order to elucidate the delocalization of electron density within the molecule.

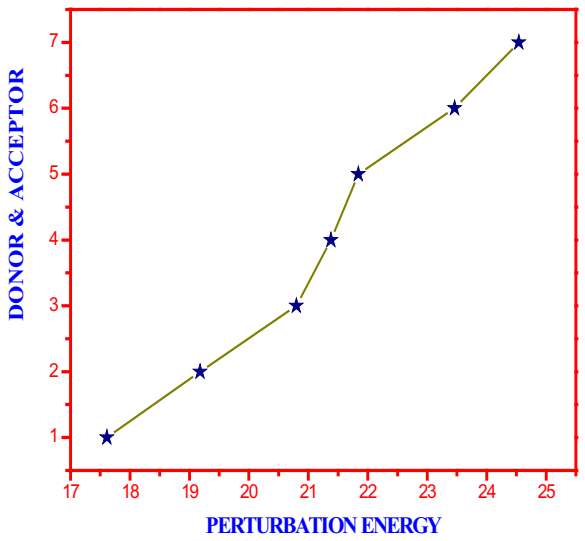
Table 4: Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis of O-Nitrobenzamide Using DFT/B3PW91/aug-cc-pVDZ Method

DONOR	BONDING	OCCUPANCY	ACCEPTOR	BONDING	OCCUPANCY	E(2) [a]Kcal/mol	ENERGY DIFFERENCE[b] E(j)-E(i) a.u	POLARISATION[c] F(I,j) a.u
C1 – C2	σ	1.97259	C1 - C6	σ*	0.01561	2.19	1.31	0.048
C1 – C2	σ	1.97259	C1 – H7	σ*	0.01402	1.00	1.16	0.031
C1 – C2	σ	1.97259	C2 – C3	σ*	0.03055	5.03	1.31	0.073
C1 – C2	σ	1.97259	C3 – C11	σ*	0.07664	3.31	1.15	0.056
C1 – C2	σ	1.97259	C6 – H10	σ*	0.01331	2.44	1.17	0.048
C1 – C2	σ	1.97259	N16 – O18	σ*	0.06567	2.35	1.16	0.047
C1 – C2	π	1.64765	C3 – C4	π*	0.32605	21.84	0.30	0.073
C1 – C2	π	1.64765	C5 – C6	π*	0.31571	17.61	0.30	0.065
C1 – C2	π	1.64765	N16 – O17	π*	0.61356	24.54	0.15	0.058
C1 – C6	σ	1.97371	C1 – C2	σ*	0.02168	2.66	1.28	0.052
C1 – C6	σ	1.97371	C1 – H7	σ*	0.01402	1.16	1.15	0.033
C1 – C6	σ	1.97371	C2 – N16	σ*	0.10480	4.71	1.00	0.063
C1 – C6	σ	1.97371	C5 – C6	σ*	0.01634	2.20	1.29	0.048
C1 – C6	σ	1.97371	C5 – H9	σ*	0.01313	2.57	1.15	0.049
C1 – C6	σ	1.97371	C6 – H10	σ*	0.01331	0.79	1.15	0.027
C1 – H7	σ	1.97520	C1 – C2	σ*	0.02168	4.28	1.30	0.067
C1 – H7	σ	1.97520	C2 – C3	σ*	0.03055	3.21	1.30	0.058
C2 – C3	σ	1.96746	C1 – C2	σ*	0.02168	4.28	1.30	0.067
C2 – C3	σ	1.96746	C1 – H7	σ*	0.01402	2.01	1.17	0.043
C2 – C3	σ	1.96746	C3 – C4	σ*	0.02115	3.21	1.30	0.058
C2 – C3	σ	1.96746	C3 – C11	σ*	0.07664	1.87	1.15	0.042
C2 – C3	σ	1.96746	C4 – H8	σ*	0.01339	2.49	1.17	0.048
C2 – C3	σ	1.96746	C11 – N12	σ*	0.07227	0.66	1.20	0.025
C3 – C4	σ	1.96320	C2 – C3	σ*	0.03055	3.83	1.29	0.063
C3 – C4	σ	1.96320	C2 – N16	σ*	0.10480	5.13	1.00	0.065

C3 – C4	σ	1.96320	C3 – C11	σ*	0.07664	1.58	1.13	0.038
C3 – C4	σ	1.96320	C4 – C5	σ*	0.01578	2.25	1.29	0.048
C3 – C4	σ	1.96320	C4 – H8	σ*	0.01339	0.76	1.15	0.026
C3 – C4	σ	1.96320	C5 – H9	σ*	0.01313	2.29	1.15	0.046
C3 – C4	σ	1.96320	C11 – O15	σ*	0.06733	1.72	1.21	0.041
C3 – C4	π	1.64566	C1 – C2	π*	0.36828	20.80	0.28	0.069
C3 – C4	π	1.64566	C5 – C6	π*	0.31571	21.38	0.29	0.070
C3 – C11	σ	1.96681	C1 – C2	σ*	0.02168	3.42	1.22	0.058
C3 – C11	σ	1.96681	C2 – C3	σ*	0.03055	1.93	1.24	0.044
C3 – C11	σ	1.96681	C2 – N16	σ*	0.10480	0.51	0.94	0.020
C3 – C11	σ	1.96681	C3 – C4	σ*	0.02115	1.80	1.22	0.042
C3 – C11	σ	1.96681	C4 – C5	σ*	0.01578	3.14	1.23	0.056
C3 – C11	σ	1.96681	N12 – H13	σ*	0.01077	3.18	1.08	0.053
C4 – C5	σ	1.97703	C3 – C4	σ*	0.02115	2.64	1.28	0.052
C4 – C5	σ	1.97703	C3 – C11	σ*	0.07664	3.23	1.13	0.055
C4 – C5	σ	1.97703	C4 – H8	σ*	0.01339	0.98	1.15	0.030
C4 – C5	σ	1.97703	C5 – C6	σ*	0.01634	2.19	1.29	0.048
C4 – C5	σ	1.97703	C5 – H9	σ*	0.01313	0.79	1.15	0.027
C4 – C5	σ	1.97703	C6 – H10	σ*	0.01331	2.64	1.15	0.049
C4 – H8	σ	1.97861	C2 – C3	σ*	0.03055	4.70	1.11	0.065
C4 – H8	σ	1.97861	C5 – C6	σ*	0.01634	3.99	1.11	0.059
C5 – C6	σ	1.97843	C1 – C6	σ*	0.01561	2.21	1.30	0.048
C5 – C6	σ	1.97843	C1 – H7	σ*	0.01402	2.75	1.15	0.050
C5 – C6	σ	1.97843	C4 – C5	σ*	0.01578	2.19	1.29	0.048
C5 – C6	σ	1.97843	C4 – H8	σ*	0.01339	2.67	1.14	0.049
C5 – C6	σ	1.97843	C5 – H9	σ*	0.01313	0.82	1.15	0.027
C5 – C6	σ	1.97843	C6 – H10	σ*	0.01331	0.88	1.15	0.028
C5 – C6	π	1.63520	C1 – C2	π*	0.36828	23.46	0.28	0.073
C5 – C6	π	1.63520	C3 – C4	π*	0.32605	19.18	0.29	0.067
C5 – H9	σ	1.98059	C1 – C6	σ*	0.01561	3.99	1.11	0.060
C5 – H9	σ	1.98059	C3 – C4	σ*	0.02115	4.27	1.10	0.061
C5 – H9	σ	1.98059	C4 – C5	σ*	0.01578	0.62	1.11	0.023
C5 – H9	σ	1.98059	C5 – C6	σ*	0.01634	0.58	1.11	0.023
C6 – H10	σ	1.98073	C1 – C2	σ*	0.02168	4.01	1.10	0.059
C6 – H10	σ	1.98073	C4 – C5	σ*	0.01578	3.98	1.11	0.059
N12 – H13	σ	1.98514	C3 – C11	σ*	0.07664	4.52	1.07	0.063
N12 – H14	σ	1.98229	C11 – O15	σ*	0.06733	3.76	1.16	0.060
N16 – O17	π	1.98546	C1 – C2	π*	0.36828	3.06	0.47	0.037
N16 – O17	π	1.98546	N16 – O17	π*	0.61356	7.21	0.33	0.052
N12	n	1.75299	C11 – O15	σ*	0.06733	5.75	0.79	0.063
O15	n	1.97717	C3 – C11	σ*	0.07664	2.13	1.09	0.044
O15	n	1.97717	C11 – N12	σ*	0.07227	2.42	1.14	0.047
O15	n	1.84949	C3 – C4	π*	0.32605	0.95	0.26	0.015
O17	n	1.98106	C2 – N16	σ*	0.10480	4.42	1.10	0.064
O17	n	1.98106	N16 – O18	σ*	0.06567	2.59	1.24	0.051
O18	n	1.97978	C2 – N16	σ*	0.10480	4.71	1.10	0.066
O18	n	1.97978	N16 – O17	σ*	0.06130	2.03	1.24	0.045
O18	n	1.88917	C11 – O15	π*	0.22113	1.82	0.43	0.026
O18	n	1.88917	N16 – O17	π*	0.61356	1.13	0.17	0.014

LP – Lone pair. [a] Stabilisation (delocalisation) energy. [b] Energy difference between i(donor) and j(acceptor) NBO orbitals. [c] Fock matrix element i and j NBO orbitals.

The intra molecular hyper conjugative interactions of π (C1–C2) to π* (N16–O17) leads to highest stabilization of 24.54 kcal mol^{-1}. In case of π (C1–C2) orbital the π*(C3–C4) shows the stabilization energy of 21.84 and 17.61 kcal mol^{-1}. Similarly in the case of π (C3–C4) to π* (C1–C2) and π* (C5–C6) anti-bonding orbital leads to stabilization energy of 20.80 and 21.38 kcal mol^{-1} and from π (C5–C6) to π* (C1–C2), π*(C3–C4) has stabilization energies of 23.46 and 19.18 kcal mol^{-1}, respectively are listed in Table 4. The π – π* transition and corresponding perturbation energy are shown in figure 4.



Note:

1=C1-C2→ C5-C6, 2=C5-C6 → C3-C4, 3=C3-C4→C1-C2, 4=C3-C4 →C5-C6, 5=C1-C2→ C3-C4, 6=C5-C6 →C1-C2, 7=C1-C2→ N16-O17

Figure 4: $\pi - \pi^*$ Transition and Corresponding Perturbation Energy

NMR Assessment

NMR spectroscopy is currently used for the structural elucidation of complex molecules. The combined use of experimental and computational tools offers a powerful gadget to interpret and predict the structure of bulky molecules. The optimized structure of o-nitrobenzamide is used to obtain the NMR spectra supported by the GIAO method with B3LYP functional at the cc-pVDZ basic set, and the chemical shifts of the compound are reported in ppm relative to TMS for ^{1}H and ^{13}C NMR spectra, which are presented in Table 5. The corresponding spectrum is shown in Fig. 5 & 6.

^{13}C NMR chemical shifts for similar organic molecules usually are >100 ppm [38, 39]. The accuracy ensures reliable interpretation of spectroscopic parameters. In the case of o-nitrobenzamide, the chemical shifts of C1, C2, C3, C4, C5, C6, and C11 are 132.429, 144.929, 122.479, 120.791, 118.984, 122.882 and 179.985 ppm respectively. The shift is higher in C2 and C11 than the others.

All the carbon atoms in the molecule are found to have higher chemical shifts due to the presence of highly negative atoms attached to the carbons. Among this C11 atom has higher chemical shift compared to all other atoms. It is due to attachment of electrons withdrawal amide carbonyl functional group.

The calculated values are compared with the experimental values. It is found that the calculated values are higher than the experimental values. And the lower peaks of hydrogen in experimental spectrum is found to be missing.

Table 5: Experimental and Calculated ^{1}H and ^{13}C NMR chemical shifts (ppm) of O-Nitrobenzamide

Atom position	Experimental Value (ppm)	Gas	Solvent		
			Methanol	Ethanol	DMSO
		B3LYP/cc-pVDZ GIAO (ppm)	B3LYP/cc-pVDZ GIAO (ppm)	B3LYP/cc-pVDZ GIAO (ppm)	B3LYP/cc-pVDZ GIAO (ppm)
C1	133	132.429	133.586	133.564	133.608
C2	147	144.929	144.798	144.797	144.8
C3	131	122.479	122.946	122.94	122.952
C4	128	120.791	122.979	122.937	123.021
C5	123	118.984	122.424	122.366	122.481
C6	132	122.882	125.152	125.114	125.188
C11	168	179.985	182.813	182.769	182.855
7H	-	6.7288	6.7987	6.7978	6.7995
8H	8.2	8.5839	8.7702	8.7671	8.7733
9H	7.6	7.554	7.8743	7.8691	7.8794
10H	7.8	7.637	7.9422	7.9374	7.9468
13H	-	2.8879	3.1966	3.1932	3.1999
14H	-	2.1573	2.6503	2.6419	2.6586

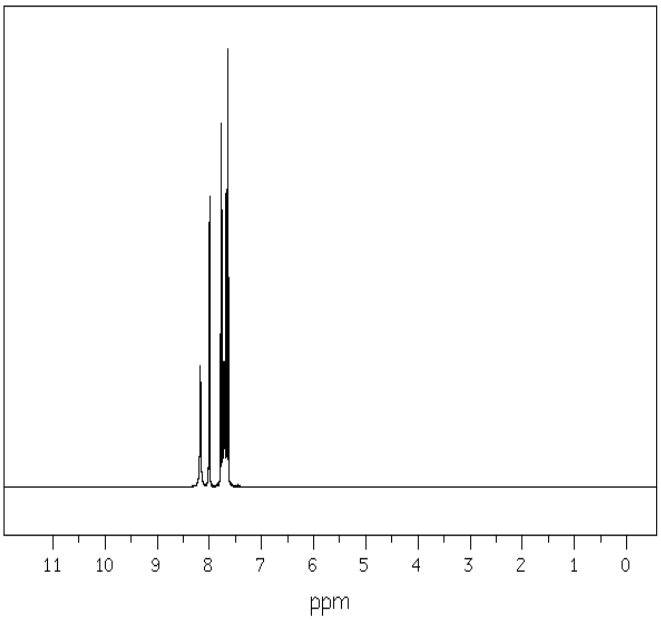


Figure 5: ^{1}H NMR Spectrum of O-Nitrobenzamide

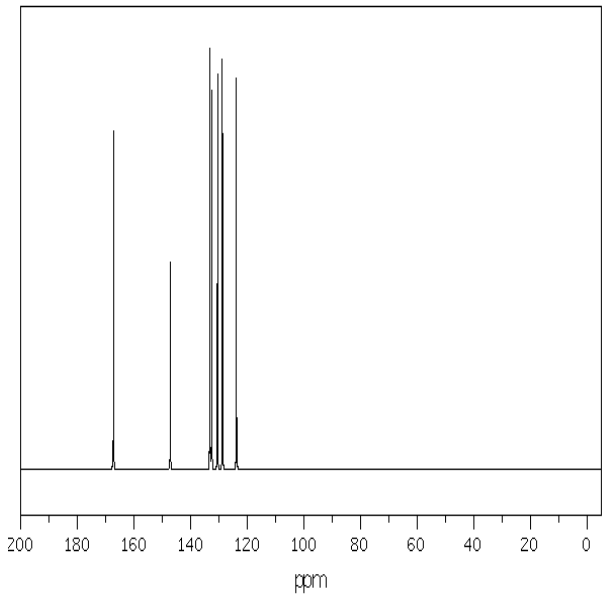


Figure 6: ^{13}C NMR Spectrum of O-Nitrobenzamide

Electronic and Optical Properties (HOMO-LUMO Analysis)

UV-visible spectroscopy is used to detect the presence of chromophores in the molecule. The calculations of the electronic structure of o-nitrobenzamide have been optimized in the singlet state. The 3D plots of frontier orbitals for the molecule are shown in Fig. 7. The low energy electronic excited states of the molecule are calculated at the B3LYP/cc-pVDZ level using the TD-DFT approach based on the previously optimized ground-state geometry of the molecule. The calculations have been performed for o-nitrobenzamide in the gas phase and with the solvent of DMSO, ethanol, and methanol. The calculated excitation energies, oscillator strength (*f*), wavelength (*λ*) and spectral assignments are presented in Table 6.

Table 6: Theoretical electronic absorption spectra of O-Nitrobenzamide (absorption wavelength λ (nm), excitation energies E (eV) and oscillator strengths (f)) using TD-DFT/B3LYP/cc-pVDZ method

λ (nm)	E (eV)	(f)	Major contribution	Assignment	Region	Bands
Gas						
341.81	3.6273	0.0128	H→L (100%)	n→π*	Quartz UV	R-band (German, radikalartig)
325.36	3.8106	0.0038	H→L (20%)	n→π*	Quartz UV	
289.07	4.2891	0.0030	H→L (15%)	n→π*	Quartz UV	
DMSO						
337.04	3.6786	0.0174	H→L (80%)	n→π*	Quartz UV	R-band (German, radikalartig)
318.58	3.8917	0.0087	H→L (40%)	n→π*	Quartz UV	
287.98	4.3053	0.0251	H→L (100%)	n→π*	Quartz UV	
Ethanol						
337.15	3.6774	0.0169	H→L (80%)	n→π*	Quartz UV	R-band (German, radikalartig)
318.75	3.8897	0.0082	H→L (40%)	n→π*	Quartz UV	
287.94	4.3059	0.0231	H→L (100%)	n→π*	Quartz UV	
Methanol						
337.03	3.6787	0.0166	H→L (80%)	n→π*	Quartz UV	R-band (German, radikalartig)
318.63	3.8912	0.0081	H→L (40%)	n→π*	Quartz UV	
287.90	4.3064	0.0229	H→L (95%)	n→π*	Quartz UV	

H: HOMO; L: LUMO

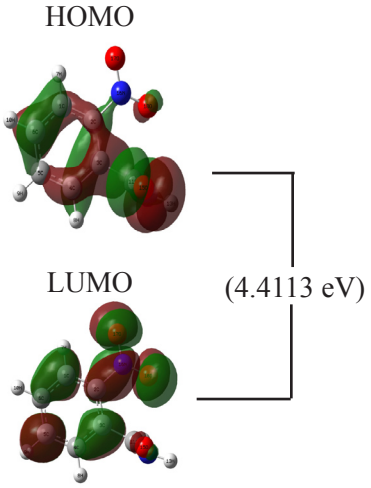


Figure 7: Frontier Molecular Orbitals of O-Nitrobenzamide

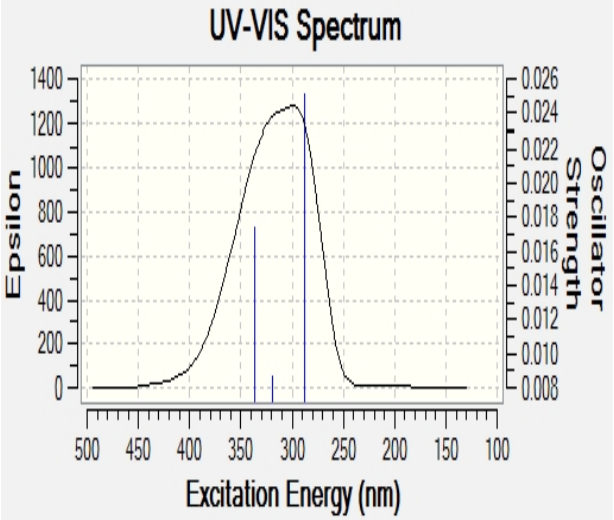


Figure 8: UV-Visible Spectrum of O-Nitrobenzamide

TD-DFT calculations predict three transitions in the quartz ultraviolet region. In the case of the gas phase, the strong transition is at 341.81, 325.36 and 289.07 nm with an oscillator strength of f = 0.0128, 0.0038, 0.0030 with 3.6273 eV energy gap. The transition is n→π* in the visible and the quartz ultraviolet region. The designation of the band is R-band (German, radikalartig) which is attributed to the above-said transition of amide groups. They are characterized by low molar absorptivities (ξ_{max}<100) and undergo a hypsochromic shift with an increase in the solvent polarity. The simulated UV-Visible spectrum of o-nitrobenzamide is shown in Fig. 8. The longer wavelengths observed on the UV spectra are due to transition from non-bonding lone pair's nitrogen and oxygen; they do have less frequency and higher perturbation energy.

In the case of the DMSO solvent, the strong transitions are obtained at 337.04, 318.58, 287.98 nm with an oscillator strength of f = 0.0174, 0.0087, 0.0251 and with a maximum energy gap of 3.6786 eV. They are assigned to n → π* transitions. This shows that, from the gas to the solvent phase, the transitions moved from the visible to the quartz ultraviolet region. This view indicates that the o-nitrobenzamide molecule has crystal property, and thus having rich NLO properties. In addition to that, the calculated optical band gap 4.4673 eV ensures that the present compound has NLO properties. In the view of calculated absorption spectra, the maximum absorption wavelength corresponds to the electronic transition from the HOMO to LUMO with maximum contribution.

Table 7: HOMO, LUMO, Kubo gap, global electronegativity, global hardness and softness, global electrophilicity index of O-Nitrobenzamide

Parameters	Gas	DMSO	Ethanol	Methanol
E_{HOMO} (eV)	-7.0167	-7.1383	-7.1340	-7.1361
E_{LUMO} (eV)	-2.6054	-2.6710	-2.6686	-2.6697
$\Delta E_{HOMO} - E_{LUMO\ gap}$ (eV)	-4.4113	-4.4673	-4.4654	-4.4664
Chemical hardness(η)	2.2056	2.2336	2.2327	2.2332
Global softness(σ)	0.4533	0.4477	0.4478	0.4477
Electronegativity(χ)	4.8110	4.9046	4.9013	4.9029
Electrophilicity index(ω)	5.2469	5.3847	5.3797	5.3820

The chemical hardness, potential, electronegativity and electrophilicity index are calculated and their values are shown in Table 7. The chemical hardness is a good indicator of the chemical stability. The chemical hardness increased slightly (2.205–2.233 eV) in going from the gas to the solvent phase. Hence, the present compound has high chemical stability. Similarly, the electronegativity is observed to have increased from 4.8 to 4.9 eV. The electrophilicity index is a measure of energy lowering due to the maximal electron flow between the donor [HOMO] and the acceptor [LUMO]. From Table 7, it is found that the electrophilicity index

of o-nitrobenzamide is 5.2469 eV in the gas phase and 5.3847 eV in solvent phase, which is moderate, and this value ensures the energy transformation between HOMO and LUMO. The dipole moment in a molecule is another important electronic property. Whenever the molecule has larger dipole moment, the intermolecular interactions are very strong. The calculated dipole moment value for the title compound is 4.9575 D in the gas phase and 6.2624 D in the solvent phase. It is high, which shows that the o-nitrobenzamide molecule has strong intermolecular interactions.

Global Softness and Local Region Selectivity

Molecular charge distribution, molecular orbital surfaces, HOMO and LUMO energies have been used as reactivity descriptors in the DFT study. The energy gap between the HOMO and LUMO orbitals has been found to be adequate to study the stability and chemical reactivity of a great variety of molecular systems and is an important stability index. Besides the traditional reactivity descriptors, there are a set of chemical reactivity descriptors that can be derived from DFT, such as global hardness (η), global softness, local softness (S), Fukui function (f), global and local electrophilicity indexes (ω).[40–50] These quantities are often defined by Koopman's theorem.[51,52]

Electronegativity (χ) is the measure of the power of an electron or a group of atoms to attract electrons towards it [53] and according to Koopman's theorem, it can be estimated using the following equation:

$$\chi = -\frac{1}{2}(E_{Homo} + E_{Lumo}) \quad (1)$$

where E_{Homo} is the energy of the highest occupied molecular orbital (HOMO) and E_{Lumo} is the energy of the lowest unoccupied molecular orbital (LUMO). Global hardness (η) measures the resistance of an atom to a charge transfer [54] and it is estimated using the equation:

$$\eta = -\frac{1}{2}(E_{Homo} - E_{Lumo}) \quad (2)$$

Global softness (S) describes the capacity of an atom or a group of atoms to receive electrons [55] and it is estimated using the equation:

$$S = \frac{1}{\eta} = -2(E_{Homo} - E_{Lumo}) \quad (3)$$

where η is the global hardness values. The global electrophilicity index (ω) is estimated using the electronegativity and chemical hardness parameters through the equation:

$$\omega = \frac{\chi}{2\eta} \quad (4)$$

A high value of electrophilicity describes a good electrophile, while a small value of electrophilicity describes a good nucleophile.

Table 8: Fukui Function and Global and Local Softness and Electrophilicity Index of O-Nitrobenzamide

Atom	f+ = (q+1)-q	f- = q-(q-1)	Δf = (f+)-(f-)	$\Delta S = \Delta f \sigma_{gs}$	$\Delta\omega = \Delta f \omega_{gei}$
1C	0.029098	0.016798	0.012300	0.00557559	0.0645381
2C	0.001077	0.006884	-0.005807	-0.00263231	-0.030469329
3C	0.003745	0.005696	-0.001951	-0.00088439	-0.010236897
4C	0.026440	0.021234	0.005206	0.00235988	0.027315882
5C	0.039029	0.031642	0.007387	0.00334853	0.038759589
6C	0.027700	0.022167	0.005533	0.00250811	0.029031651
7H	0.042211	0.054621	-0.012410	-0.00562545	-0.06511527
8H	0.047403	0.055193	-0.007790	-0.00353121	-0.04087413
9H	0.059105	0.064098	-0.004993	-0.00226333	-0.026198271
10H	0.055008	0.061720	-0.006712	-0.00304255	-0.035217864
11C	0.062395	0.055484	0.006911	0.00313276	0.036262017
12N	0.067579	0.012124	0.055455	0.02513775	0.290972385
13H	0.046722	0.035364	0.011358	0.00514858	0.059595426
14H	0.045745	0.031938	0.013807	0.00625871	0.072445329
15O	0.095817	0.011028	0.084789	0.03843504	0.444889982
16N	0.003696	0.059376	-0.055680	-0.02523974	-0.29215296
17O	0.185714	0.221245	-0.035531	-0.0161062	-0.186431157
18O	0.161491	0.233389	-0.071898	-0.03259136	-0.377248806

ΔS = local softness, σ_{gs} = global softness; **Δω** = local electrophilic index, ω_{gei} = global electrophilic index.

Fukui indices is a measure of the chemical reactivity, as well as an indicator of the reactive regions and the nucleophilic and electrophilic behaviors of the molecule. The regions of a molecule, where the Fukui function is large, are chemically softer than the regions where the Fukui function is small, and by invoking the HSAB principle in a local sense, one may establish the behavior of different sites with respect to hard or soft reagents. The Condensed to atom Fukui function is a reactive descriptor to identify nucleophilic and electrophilic attack sites in candidate molecules; perhaps it is also used to recognize the electron acceptor center and donor centers. If *fk*+ for any given site is positive then it is a preferred site for nucleophilic attack, in contrast the negative value implies electrophilic attack.

The Fukui function is defined as [56, 57]:

$$f(r) = \left(\frac{\partial \rho(r)}{\delta N}\right)_{v(r)} \quad (5)$$

Where $\rho(r)$ is the electron density and

$$N = \int \rho(r)\mathrm{d}r \quad (6)$$

Where N is the number of electrons and r is the external potential exerted by the nucleus.

The phenyl ring gets activated at the *ortho* and *para* positions as there are electron releasing substituents such as –OH, –NH_2, –OR, R, etc. A propyl substituent in fact is an electron releasing substituent, consequently promotes the *ortho* and *para* positions for electrophilic attack, a common reactivity trend observed in phenyl compounds. Local reactivity descriptors such as *fk*+, *fk*-, Δf, ΔS and $\Delta\omega$ for the different sites of the phenyl ring are in conformity with the observed reactivity trend of the candidate molecule. The values are shown in Table 8.

fk+, *fk*-, Δf, ΔS and $\Delta\omega$ unambiguously reveal the order of the nucleophilic attack to be in the decreasing sequence as C1 > C5 > C11>C6>C4 and that of the electrophilic attack is found to be C3 > C2 in the phenyl ring. This trend for the attack of the electrophile is in conformity with that of ΔS and $\Delta\omega$. The atoms C2, C3 are more prone to nucleophilic attack and C1, C5 are more favorable to electrophilic attack. The *ortho* and *para* positions show the tendency for attack of the electrophile, which is indeed a common trend observed in alkyl substituted phenyl ring compounds. The different charges of atoms are plotted and shown in the fig. 9 & 10.

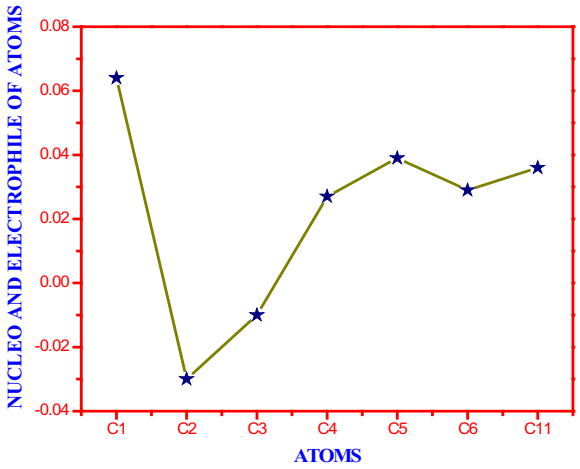


Figure 9: Positively & Negatively Charged Atoms of O-Nitrobenzamide Using Fukui Function

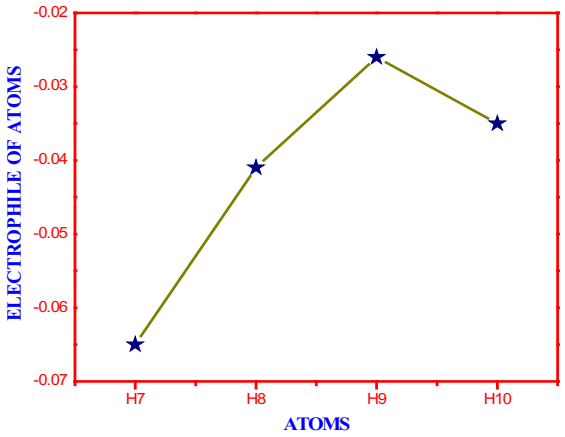


Figure 10: Negatively Charged Atoms ofO-Nitrobenzamide Using Fukui function

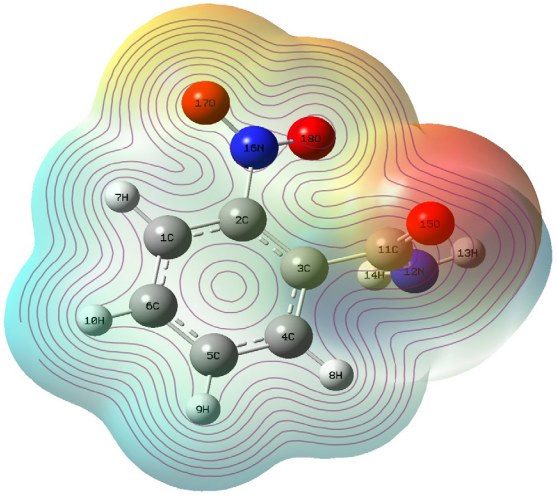


Figure 11: MEP Contour Map of O-Nitrobenzamide

Molecular Electrostatic Potential (MEP) Maps

The molecular electrical potential surfaces, as shown in Fig. 11, illustrate the charge distributions of molecules three dimensionally. This map allows visualizing variably charged regions of a molecule. The knowledge of the charge distributions can be used to determine how molecules interact with one another and it is also used to determine the nature of the chemical bond. Molecular electrostatic potential is calculated at the B3LYP/cc-pVDZ optimized geometry. [58, 59] There is a great deal of intermediary potential energy, and the non-red or blue regions indicate that the electro negativity difference is not very great. In a molecule with a great electro negativity difference, charge is very polarized, and there are significant differences in electron density in different regions of the molecule. This great electro negativity difference leads to regions that are almost entirely red and almost entirely blue. [60] The Greater regions of intermediary potential, yellow and green, and smaller or no regions of extreme potential, red and blue, are key indicators of smaller electronegativity.

The color code of these maps is in the range between –5.490 a.u. (deepest red) and 5.490 a.u. (deepest blue) in the compound. The positive (blue) regions of MEP are related to electrophilic reactivity and the negative (green) regions to nucleophilic reactivity (Fig. 11). From the MEP map of the candidate molecule, it can be observed that the red regions of the molecule were found to be ready for electrophilic attack, and especially in the phenyl ring the atoms are clouded with red color. From the findings of the Fukui local reactivity descriptor, it can be observed that the atoms C1, C4, C5, C6 and C11 are nucleophiles ready for electrophilic attack and atoms C2 and C3 are the regions for nucleophilic attack. The molecular electrostatic potential map can be confirmed with the finding of the Fukui descriptors.

Polarizability and First Order Hyperpolarizability Calculations

In order to investigate the relationships among molecular structures and non-linear optic properties (NLO), the polarizabilities and first order hyperpolarizabilities of the o-nitrobenzamide compound were calculated using the DFT-B3LYP method and the cc-pVDZ basis set, based on the finite-field approach.

The polarizability and hyperpolarizability tensors (α_{xx}, α_{xy}, α_{yy}, α_{xz}, α_{yz}, α_{zz} and β_{xxx}, β_{xxy}, β_{xyy}, β_{yyy}, β_{xxz}, β_{xyz}, β_{yyz}, β_{xzz}, β_{yzz}, β_{zzz}) can be obtained by a frequency job output file of Gaussian. However, α and β values of the Gaussian output are in atomic units (a.u.); so they have been converted into electronic units (esu) (α, 1 a.u. = 0.1482×10^{-24} esu; β, 1 a.u. = 8.6393×10^{-33} esu). The calculations of the total molecular dipole moment (μ), linear polarizability (α) and first-order hyperpolarizability (β) from the Gaussian output have been explained in detail previously,[61,62] and DFT has been extensively used as an effective method to investigate the organic NLO materials.[63–67]

$$\alpha_{tot} = \frac{1}{3}(\alpha_{XX} + \alpha_{YY} + \alpha_{ZZ})$$

$$\Delta\alpha = \frac{1}{\sqrt{2}}\left[\begin{matrix}(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 \\ +(\alpha_{zz} - \alpha_{xx})^2 + 6\alpha^2_{xz} + 6\alpha^2_{xy} + 6\alpha^2_{yz}\end{matrix}\right]^{\frac{1}{2}}$$

$$\langle\beta\rangle = \left[\begin{matrix}(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yzz} + \beta_{yxx})^2 \\ +(\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2\end{matrix}\right]^{\frac{1}{2}}$$

Table 9: The electronic dipole moment (μ) (Debye), polarizability (α) and first hyperpolarizability (β) of O-Nitrobenzamide

Parameter	a.u.	Parameter	a.u.
α_{xx}	-55.5541	β_{xxx}	-36.4230
α_{xy}	5.2440	β_{xxy}	7.8514
α_{yy}	-71.4564	β_{xyy}	1.0538
α_{xz}	3.4014	β_{yyy}	19.7313
α_{yz}	0.1110	β_{xxz}	-3.0686
α_{zz}	-69.7811	β_{xyz}	3.2892
α_{tot}	-65.5972	β_{yyz}	-1.6681
$\Delta\alpha$	13.1587	β_{xzz}	-10.9696
μ_x	-1.9888	β_{yzz}	-7.4288
μ_y	- 5.7088	β_{zzz}	-1.9797
μ_z	-0.9490	β_{tot}	50.9762
μ_{tot}	6.1193		

In Table 9, the calculated parameters described above and the electronic dipole moment $\{\mu_i\ (i = x, y, z)\}$ and total dipole moment μ_{tot} for the title compound are listed. The total dipole moment is calculated using the following equation: [68]

$$\mu_{tot} = \left(\mu^2_x + \mu^2_y + \mu^2_z\right)^{\frac{1}{2}}$$

It is well known that the molecules with high values of dipole moment, molecular polarizability, and first hyperpolarizability have more active NLO properties. The first hyperpolarizability *(β)* and the components of hyperpolarizability α_x, α_y and α_z of o-nitrobenzamide along with related properties *(α_0*, α_{total}, and *$\Delta\alpha$*) are reported in Table 8. The calculated value of the dipole moment is found to be 6.1193 D. The highest value of the dipole moment is observed for component $\mu_{Z,}$ which is equal to −0.9490 D and the lowest value of the dipole moment of the molecule for the component μ_y is −5.7088 D. The calculated average polarizability and anisotropy of the polarizability is -9.721×10^{-24} esu and 1.950×10^{-24} esu, respectively. The magnitude of the molecular hyperpolarizability is one of the important key factors in an NLO system. The B3LYP/cc-pVDZ calculated first hyperpolarizability value (β) is 4.404×10^{-35} esu. From the above results, it is observed that, the molecular polarizability and hyperpolarizability of the title compound in all coordinates are active. So that o-nitrobenzamide can be considered to the good candidate for NLO material.

Conclusion

In the geometrical study, it is observed by the calculation of the bond length and bond angle, the hexagonal structure of the compound is deformed. In the vibrational study though most of the vibrations are in line with the literature some the mode carbonyl group is shifted to the end position of the range. The NMR reveals that the C11 atom which is attached to the carbonyl and amine group has more shift compared to all other atoms in the compound; it means that atom is more deshielded by its electrons. From the UV steady it is found that the π and nonbonding orbital transitions have almost occurred in the spectra. From the range of the wavelength it is observed that the transition entered into the visible blue range. Thus it is a good candidate of the NLO material. From the MEP mapping and Fukui study the possible electrophile and nucleophile have been identified.

References

1. R.J. Knox, M.P. Boland, F. Friedlos, B. Coles, C. Southan, J.J. Roberts, Biochemical Pharmacology, 37 (1988) 4671–4677.
2. A. Chandor, S. Dijols, B. Ramassamy, Y. Frapart, D. Mansuy, D. Stuehr, N. Helsby, Chemical Research Toxicology, (2008), 21, 836–843.
3. R.J. Lewis, Sr (Ed.). Hawley's Condensed Chemical Dictionary, 12th ed. New York, NY: Van Nostrand Rheinhold Co., (1993) 860.
4. D. Hartley and H. Kidd (eds.), The Agrochemicals Handbook. Old Woking, Surrey, United Kingdom: Royal Society of Chemistry/Unwin Brothers Ltd., (1983).
5. W. Gerhartz, Ullmann's Encyclopedia of Industrial Chemistry. 5th ed: Deerfield Beach, FL: VCH Publishers, 1985.
6. M.K. Marchewka, A. Pietraszko, Spectrochimica Acta Part A, 69 (2008) 312– 318.
7. M.J. Frisch, Gaussian 09, Revision A.02, Gaussian, Inc., Wallingford CT, 2009.
8. Z. Zhengyu, D. Dongmei, Journal of Molecular Structure, 505 (2000) 247-252.
9. Z. Zhengyu, F. Aiping, D. Dongmei, Journal of Quantum Chemistry, 78 (2000) 186-189.
10. A.D. Becke, Physics Review A, 38 (1988) 3098-3101.
11. C. Lee, W. Yang, R.G. Parr, Physics Review B, 37 (1988) 785-790.
12. A.D. Becke, Journal of Chemical Physics, 98 (1993) 5648-5652.
13. R.L. Peesole, L.D. Shield, I.C. McWilliam, Modern Methods of Chemical Analysis, Wiley, New York, 1976.
14. S. Mohan, N. Sundaraganesan, J. Mink, Spectrochim. Acta A, 47 (1991) 1111–1115.
15. G.N. Ten, V.V. Nechaev, A.N. Pankratov, V.I. Berezin, V.I. Baranov, *Journal* of Structural *Chemistry*, 51 (2010) 854–861.
16. V. Arjunan, S. Sakiladevi, T. Rani, C.V. Mythili, S. Mohan, Spectrochimica Acta Part A, 88 (2012) 220–231
17. C. Cırak, N. Koc, Journal of Molecular Modeling, 18 (2012) 4453–4464.

18. N.P.C. Roeges, A Guide to the Complete Interpretation of Infrared Spectra of Organic Structure, Wiley, New York, USA, 1994.
19. Y.R. Sharma, Elementary Organic Spectroscopy, Principles and Chemical Applications, S.Chande & Company Ltd., New Delhi, 1994.
20. P.S. Kalsi, Spectroscopy of Organic Compounds, Wiley Eastern Limited, New Delhi, 1993.
21. V. Karunakaran, V. Balachandran, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 98 (2012) 229 –239.
22. V. Arjunan, K. Carthigayan, S. Periandy, K. Balamurugan, S. Mohan, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 98 (2012) 156–169.
23. V. Arjunan, K. Carthigayan, S. Periandy, K. Balamurugan, S. Mohan, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 98 (2012) 156–169.
24. V. Karunakaran, V. Balachandran, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 98 (2012) 229–239.
25. M. Silverstein, G. Clayton Basseler, C. Morrill, Spectrometric identification of organic Compounds, John Wiley, New York, 1991.
26. C. Brian Smith, Infrared Spectral Interpretation, CRC Press, New York, 1999.
27. G. Socrates, Infrared and Raman Characteristics Group Frequencies, Wiley, New York, 2000.
28. M. Silverstein, G. Clayton Basseler, C. Morill, Spectrometric Identification of Organic Compound, Wiley, New York, 1981.
29. R. Shanmugam, D. Sathyanarayana, Spectrochim. Acta A, 40 (1984) 764.
30. A. Prabakaran, S. Muthu, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 118 (2014) 578–588.
31. R. Zhang, X. Li, X. Zhang, Frontiers of Chemistry in China, 6 (2011) 358-366.
32. K. Carthigayan, V. Arjunan, R. Anitha, S. Periandy, S. Mohan, Journal of Molecular Structure, 1056 (2014) 38–51.
33. S. Subhashandrabose, R. Akhil, R. Krishnan, H. Saleem, R. Parameswari, N. Sundaraganesan, V. Thanikachalam, G. Manikandan, Spectrochim. Acta, 77A (2010) 877–884.
34. J.N. Liu, Z.R. Chen, S.F. Yuan, Journal of Zhejiang University-Science B, 6 (2005) 584–589.
35. C. James, A. Amalraj, A. Regunathan, V.S. Jayakumar, I.H. Joe, Journal of Raman Spectroscopy, 37 (2006) 1381–1392.
36. A.R. Krishanan, H. Saleem, S. Subhashandrabose, N. Sundaraganesan, S. Sebastian, Spectrochimica. Acta A, 78 (2011) 582–589.
37. S. Sebastian, N. Sundaraganesan, Specrochim. Acta, A 75 (2010) 941–952.
38. J.H. Vander Maas and E.T.G. Lutz, Spectrochimica Acta, A 30 (1974) 2005.
39. S. Ahmad, S. Mathew, P.K. Verma, Indian Journal of Pure and Applied Physics, 30 (1992) 764-770.
40. R.G. Parr, W. Yang, Density Functional Theory of Atoms and Molecules, Oxford University Press, New York, 1989.
41. P. Geerlings, F. De Proft, W. Langenaekar, Advanced Quantum Chemistry, 33(1999) 303-332.
42. K. Hohenberg, W. Kohn, Physical Review, 136 (1964) B864.
43. R.G. Pearson, Journal of American Chemical Society, 85 (1963) 3533-3539.
44. R.G. Parr, R.G. Pearson, Journal of American Chemical Society, 105 (1983) 7512-7516.
45. R.G. Parr, R.A. Donnelly, M. Levy, W.E. Palke, Journal of Chemical Physics, 68 (1978) 3801-3807.
46. R.G. Pearson, Journal of American Chemical Society, 107 (1985) 6801-6806.
47. R.G. Parr, W. Yang, Journal of American Chemical Society, 106 (1984) 4049-4059.
48. R.G. Parr, L.V. Szentpaly, S. Liu, Journal of American Chemical Society, 121 (1999) 1922-1924.
49. P. Perez, A. Toro-Labbe, A. Aizman, R. Contreras, Journal of Organic Chemistry, 67 (2002) 4747-4752.

50. W. Yang, W. Mortier, Journal of American Chemical Society, 108 (1986) 5708-5711.
51. P. Geerlings, F. De Proft, W. Langenaeker, Chem. Rev. 103 (2003) 1793-1874.
52. R.G. Parr, R.G. Pearson, Journal of American Chemical Society, 105 (1983) 7512-7516.
53. L. Pauling, The Nature of the Chemical Bond (Coruell University Press, Ithaca, New York, 1960.
54. R.G. Parr, R.G. Pearson, Journal of American Chemical Society, 105 (1983) 7512-7516.
55. R.G. Parr, W. Yang, Functional Theory of Atoms and Molecules, Oxford University Press, New York, 1989.
56. P.W. Ayers, R.G. Parr, Journal of American Chemical Society, 122 (2000) 2010-2018.
57. R.G. Parr, W. Yang, Journal of American Chemical Society, 106(1984) 4048- 4049.
58. M. Nendel, K.N. Houk, L.M. Tolbert, E. Vogel, H. Jiao, P.V.R. Schleyer, Journal of Physical Chemistry. A, 102 (1998) 7191-7198.
59. C.H. Choi, M. Kertesz, Journal of Chemical Physics, 108 (1998) 6681-6688.
60. A. Vektatiene, Journal of Organic Chemistry, 26 (2009) 321-322.
61. H. Tanak, Y. Köysal, H. Yaman, V. Ahsen, Bulletin of Korean Chemical Society, 32 (2011) 678-686.
62. K.S.Thanthiriwatte, K.M. Nalin de Silva, Journal of Molecular Structure (Theochem) 617 (2002) 169-175.
63. Y.X. Sun, Q.L. Hao, Z.X. Yu, W.X. Wei, L.D. Lu, X. Wang, Molecular Physics, 107 (2009) 107, 223-235.
64. A.B. Ahmed, H. Feki, Y. Abid, H. Boughzala, C. Minot, A. Mlayah, Journal of Molecular Structure, 920 (2009) 1-4.
65. J.P. Abraham, D. Sajan, V. Shettigar, S.M. Dharmaprakash, I. Nemec, I.H. Joe, V.S. Jayakumar, Journal of Molecular Structure, 917 (2009) 27-36.
66. S.G. Sagdinc, A. Esme, Spectrochimica Acta Part A, 75 (2010) 1370-1376.
67. A.B. Ahmed, H. Feki, Y. Abid, H. Boughzala, C. Minot, Spectrochimica Acta Part A, 75 (2010) 293-298.
68. Y.J. Jiang, Chinese Science Bulletin, 57 (2012) 4449-4453.

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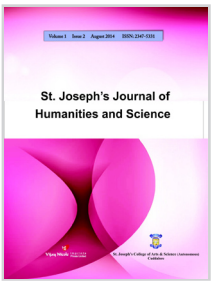

Effects of Precursor Type and Molarity on Phase Stability and Optical Properties of In_2O_3 Thin Films Deposited by Spray Pyrolysis

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Abstract

In_2O_3 thin films were deposited by spray pyrolysis using $InCl_3$ and $InNO_3$ as precursors onto glass substrate. The structural, morphological and optical characteristics have been studied with the variation of precursor concentration. XRD analysis showed the structural orientation of films especially along (222) plane. SEM and AFM studies revealed that the film deposited with 0.10M at 500°C has spherical grains with almost uniform dimension. The band gap energy, refractive index, extinction coefficient and dielectric constants were estimated from U-V absorption data. The variation of these optical parameters with precursor type and its molarity has been investigated. The intense violet light emissions for all the films except the film at 0.15M for $InCl_3$ precursor were observed in the PL spectra. It was observed that resistivity of the films decreased while carrier concentration and mobility increased compared with $InNO_3$ precursor.

Keywords: Precursor; Molarity; SEM; AFM; Transmittance.

Introduction

Highly transparent Indium oxide (In_2O_3) thin films having wide band gap are very important materials for optoelectronic and gas sensing applications due to their low resistivity and good adherence to substrates [1-3]. Among the various transparent conducting oxides, In_2O_3 has attracted immense attention due to its enormous applications in many fields, such as optoelectronic devices, thin film solar cells [4] and gas sensors [5].

In_2O_3 films have been deposited using numerous methods such as reactive evaporation [6], pulsed laser evaporation [7], sputtering [8], sol–gel technique [9], chemical vapour deposition [10] and spray pyrolysis [11] etc. Among these methods, spray pyrolysis technique offers many advantages such as the low cost of the apparatus and source materials, accurate control

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over the deposition parameters and producing large area films deposition compared to other deposition methods. In_2O_3 films were deposited so far using various precursors, including $InCl_3$, $InNO_3$, In-acetate and In-acac. Among these precursors, $InCl_3$ is a predominant and $InNO_3$ is an infrequent source material for In_2O_3 films deposition.

In the present work, comparative structural, morphological and optical characteristics of sprayed In_2O_3 films deposited from $InCl_3$ and $InNO_3$ as precursors at different molar concentrations was carried out. Initially the characterizations like XRD, SEM with EDAX of deposited films at different temperatures at a constant precursor concentration are studied and the optimum temperature was fixed for both the precursors. Then the optimum molarity was found by various studies of deposited In_2O_3 films for various precursor concentrations with this optimum temperature. The scope of this work is to optimize the molar concentration and precursor of highly transparent conductive In_2O_3 film with optimum properties.

Experimental Details

In_2O_3 films were deposited at different molarities with different precursors ($InCl_3$ and $InNO_3$) by a pneumatic controlled spray pyrolysis. The precursor and deionized water mixture was sprayed onto glass substrate with dimension of 75 x 25 mm^2. During the experiments, the precursor concentration was varied from 0.05M to 0.15M by keeping the substrate temperature and other deposition parameters as constant. In the spray pyrolysis unit, the substrate temperature was maintained with the help of a heater and an electronic circuitry, which contains a thermal sensor with relay switch. The precursor solution and career gas assembly connected to spray gun was moved in the horizontal plane by means of pneumatic controlled system. The substrate to nozzle distance was maintained at 25 cm with an angle of 45°. The films deposited on pre-cleaned glass plates were gradually cooled to room temperature and then rinsed with deionized water and dried.

The well-adherent In_2O_3 films underwent structural, morphological and optical studies. The structural study was carried out using SHIMADZU-6000 diffractometer equipped with CuKα radiation (λ=1.5418 Å). The surface morphology was examined by HITACHI, S-3400N scanning electron microscope (SEM) equipped with electron dispersive X-ray spectroscopy (EDS) and NANONICS MV 1000 atomic force microscopy (AFM). The optical and photoluminescence spectra were recorded using JASCOV-670 spectrophotometer and Plorolog3-HORIBA JOBIN-YVON, respectively.

Results and Discussion

Structural Studies

The XRD spectra of In_2O_3 films for the molarities 0.05M, 0.1M and 0.15M for the precursor (i) $InCl_3$ and precursor (optimized substrate temperature 500°C) (ii) $InNO_3$ (optimized substrate temperature 400°C) are as shown in Fig. 1. The prominent peaks are in good agreement with the JCPDS Card No-06-0416. Thus the deposited films are polycrystalline in nature with a body centered cubic (bcc) structure having Ia3 space group .The calculated lattice constant for all films is a=10.06Å, which is slightly less than the standard value 10.11 Å [12]. This slight variation of the unit cell dimension is due to tight packing of In_2O_3 cubic crystal.

For 0.05M/$InCl_3$, only (222) and (400) reflections are present. But for 0.10M/$InCl_3$, the intensity of (400) reflection is reduced and (211), (440) and (622) reflections appear with very low intensity. Only the (222) reflection is present with a very high intensity. For 0.15M/$InCl_3$, the intensity of (400) reflection is increased, with (222), (211), (440) and (622) reflections are present with slightly increased intensity.

For 0.05M/$InNO_3$, only (222) reflection is present with low intensity. But for 0.10M and 0.15M, (211), (400), (440) and (622) reflections just appear with very low intensity, except (222) reflection is present with a very high intensity.

Among the above prepared films, $InCl_3$ precursor at 0.10M has (222) plane with a very high intensity exhibiting the improved crystalline structure and also degree of film texturing, as I(222)/I(400) ratio, is observed to be maximum.

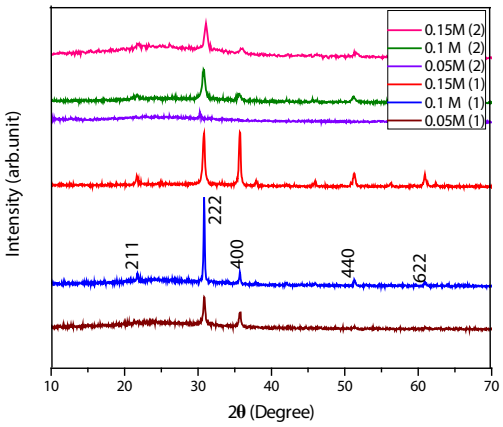


Figure 1: XRD Spectra of In_2O_3 films at Different Molarities for the Precursors (i) $InCl_3$ and (ii) $InNO_3$

The lattice parameter (a=b=c) was determined using the following equation [16]:

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (1)$$

where d is the lattice spacing of the crystal planes (h k l)

The crystallite size calculations are carried out from the Scherer-Bragg equation [13]:

$$D = \frac{k\lambda}{\beta \cos\theta} \quad (2)$$

where θ is the Bragg's angle, β is the full width at half maximum of the peaks and λ is the X-ray wave length.

The micro strain (ε) is determined with the relation:

$$\varepsilon = \frac{\beta \cos\theta}{4} \quad (3)$$

The dislocation density (δ) is calculated using the relation:

$$\delta = \frac{1}{D^2} \quad (4)$$

The inter planar spacing (d_{hkl}) is calculated using the relation

$$d_{hkl} = \frac{n\lambda}{2\sin\theta} \quad (5)$$

The above structural and micro structural parameters calculated from the (222) reflection, for different precursors/molarities are listed in Table 1. It can be noticed that the 0.10M (1) has the optimized and favorable parameters rather than other molarities, smallest micro strain and dislocations density with an average crystallite size around 18 nm.

Table.1.Grain size, Micro strain, Dislocation density and Inter-planar spacing of In_2O_3 films at different molarities for the precursors (i) $InCl_3$ and (ii) $InNO_3$

Molar Concentration	Grain size, D (nm)		Micro strain, ε x10^{-3}		Dislocation density, δ x10^{14} (m^{-2})		Inter- planar Spacing (nm)	
	(i)	(ii)	(i)	(ii)	(i)	(ii)	(i)	(ii)
0.05M	26.906	8.676	1.05	4.17	13.813	132.839	0.266	0.140
0.1 M	47.750	18.313	0.76	1.98	4.385	29.817	0.262	0.237
0.15M	27.408	14.486	1.32	2.5	13.311	47.653	0.245	0.431

Surface Morphological Studies

Fig. 2 shows SEM micrographs of In_2O_3 films with the precursors (i) $InCl_3$ and (ii) $InNO_3$ at three different molarities. For $InCl_3$ precursor, the film at 0.05M shows that the surface is filled by means of very fine grains with some irregularities and 0.10M shows the smoothened film with spherical grains. In the film surface for 0.15M, randomly oriented grains are present due to the higher molarity. For the $InNO_3$ precursor the film at 0.05M showed that the surface filled by means of small grains with some pin holes and for film 0.10M has shown smoothened film with spherical grains. The film surface for 0.15M the randomly oriented grains are present due to the higher molarity. On comparing SEM images of the two precursors, the film at 0.10M having better morphology than the other films for both precursors. Moreover, the film with $InCl_3$ precursor at 0.10M has uncluttered surface morphology. Fig. 3 contains EDS of In_2O_3 films at 0.1M for $InCl_3$ and $InNO_3$ precursors and it shows that the composition of In and O atomic ratios are 23.5: 76.5 and 14.25: 85.75 respectively.

AFM images of $InCl_3$ and $InNO_3$ precursors at 0.10M as shown in Fig. 4, confirm the results already obtained by SEM analysis. Irregular-shaped particles (close to spherical) in the nanoscale with homogeneous size distribution are observed, forming somehow smooth surface with less porosity.

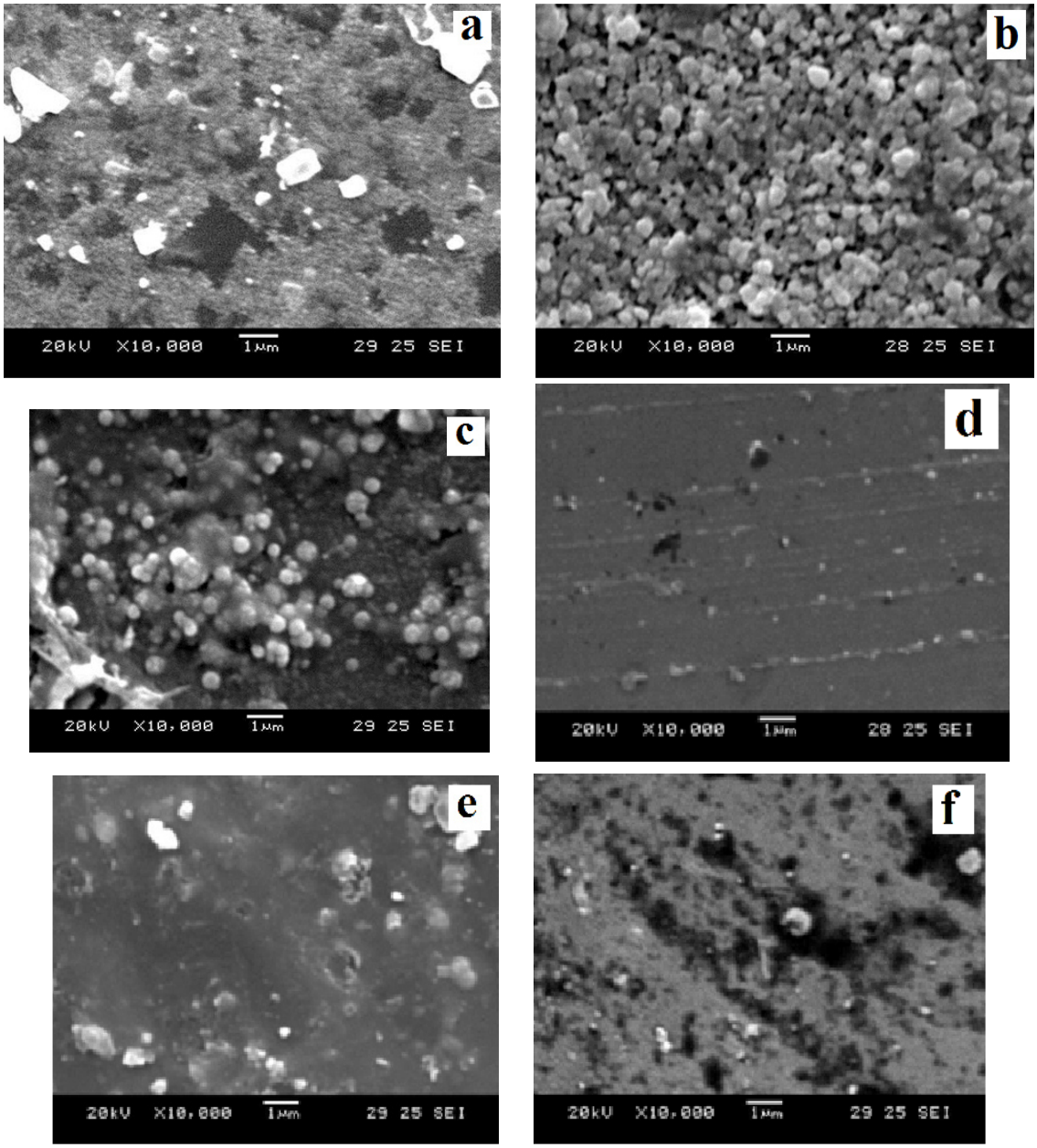
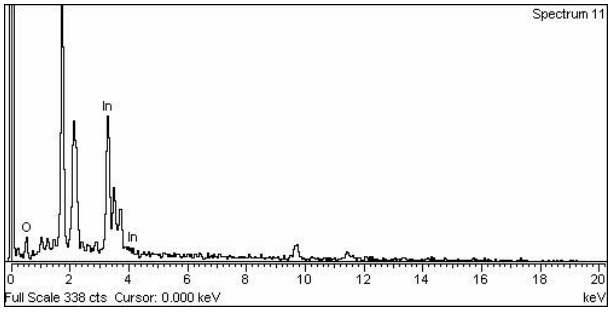
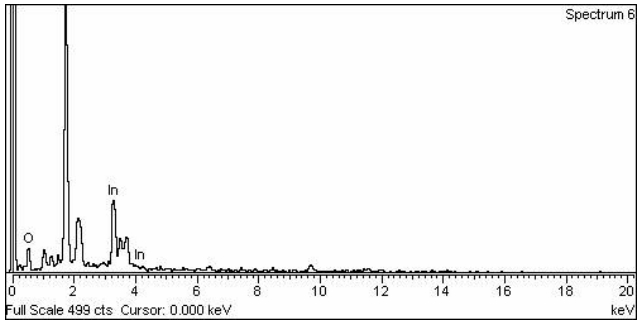


Figure 2: SEM Images of In_2O_3 films at (a) 0.05M (b) 0.1M (c) 0.15M for $InCl_3$ (d) 0.05M (e) 0.1M (f) 0.15M for $InNO_3$ Precursors.

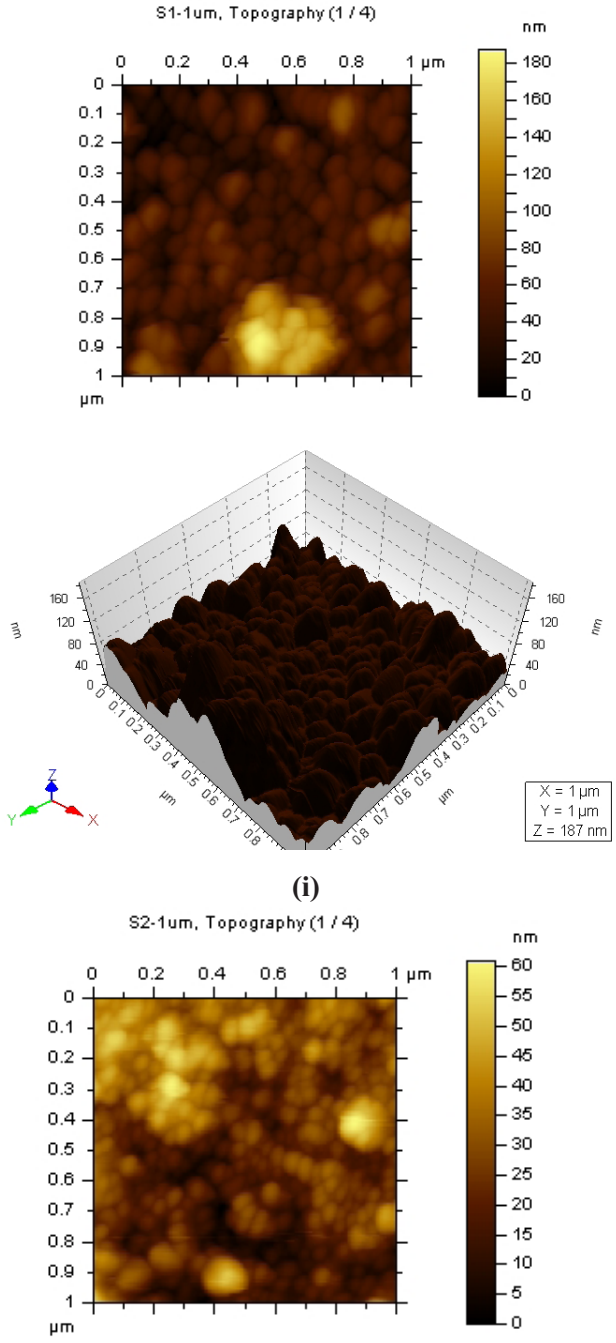


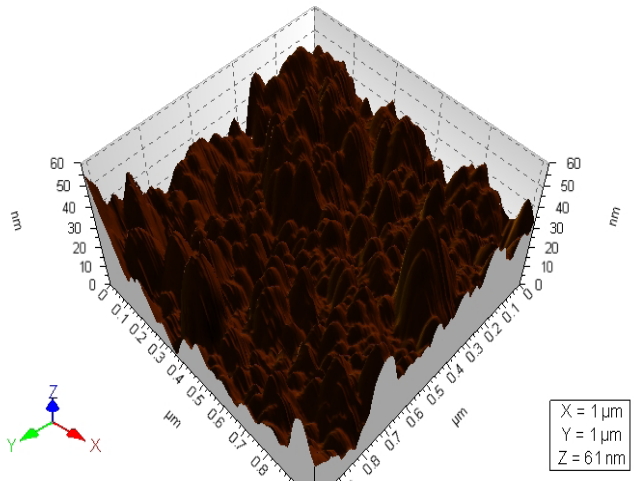
(i)



(ii)

Figure 3: EDS Spectra of In_2O_3 films at 0.1M for the Precursors (i) $InCl_3$ and (ii) $InNO_3$





(ii)

Figure 4: 2D and 3D AFM Images of the film for (i) $InCl_3$ (ii) $InNO_3$ Precursors at 0.1M

Optical Properties of In_2O_3 Films

The optical transmittance spectra of In_2O_3 films at the molarities 0.05M, 0.1M and 0.15M for the precursors (i) $InCl_3$ and (ii) $InNO_3$ are as shown in fig.5 for the wavelength range of 300 nm to 1200 nm. The percentage of transmittance for all the films is minimum in UV region and maximum in the visible and near infra-red regions. The increasing transmittance percentage is due to uniform oxidation and improved lattice arrangements [14]. From the transmittance spectra, the transmittance percentage for the films at 0.05M and for 0.1M for the $InNO_3$ precursor are maximum and the films at 0.15M for both the precursors are observed to be minimum. The transmittance percentage of the films deposited at 0.05M and 0.1M for $InCl_3$ precursor are nearly maximum and also the film at 0.1M exhibit perfect interference pattern due to well crystallinity as evident from XRD results in fig.1.

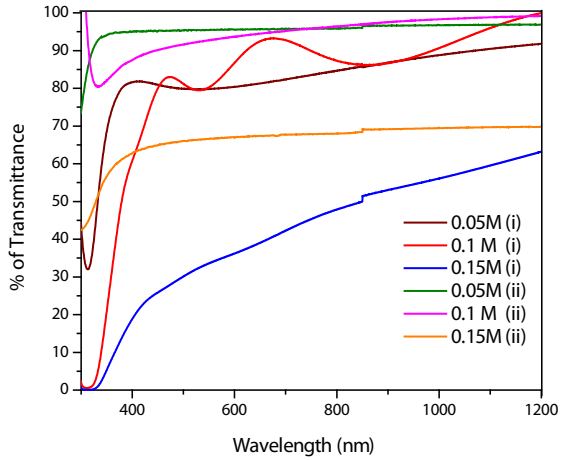


Figure 5: Optical Transmission Spectra of In_2O_3 Films at Different Molarities for the Precursors (i) $InCl_3$ and (ii) $InNO_3$

The optical band gap of deposited In_2O_3 films is evaluated from the relation between absorption coefficient α and photon energy hν [15].

$$(\alpha h\nu) = A\,(h\nu - E_g)^{x} \quad (6)$$

Where A is a constant, E_g is the optical band gap and x =1/2 for directly allowed electronic transitions. The fig.6 shows the plot between $(\alpha h\nu)^2$ and hν of the deposited films at 0.05M,0.1M and 0.15M for the precursors (i) $InCl_3$ and (ii) $InNO_3$.The extrapolation of linear portion of the curves on □ν axis gives the direct band gap energy. The spectra shows that the band gap energy of the films ranging from 3.133 eV to 3.689 eV. The increasing of band gap energy is accredited to the carrier density due to Brustein-Moss effect [16]. The high value of band gap energy for the film at 0.1M for the $InCl_3$ precursor is 3.689eV due to homogeneous and smoothened surface morphology of the film.

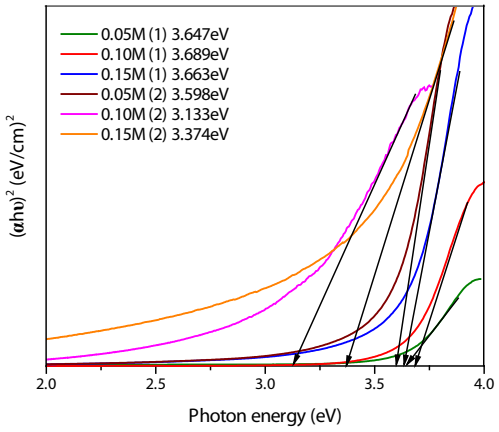


Figure 6: Optical Band Gap Spectra of In_2O_3 Films at Different Molarities for the Precursors (i) $InCl_3$ and (ii) $InNO_3$

The extinction coefficient (k) can be determined using the relation [17]

$$k = \frac{\alpha\lambda}{4\pi} \quad (7)$$

Fig.7 shows the variation of extinction coefficient with wavelength of In_2O_3 films at different molarities for the precursors (i) $InCl_3$ and (ii) $InNO_3$. In this spectra all the films having maximum k in the U-V region, almost constant and minimum in the visible and near infrared regions. Especially, the spectrum of the film at 0.1M for the $InCl_3$ precursor is revealed better disparity of k between U-V and visible regions than the other molarities and nearly zero extinction coefficient. The minimum of extinction coefficient or the index of absorption established that the films are highly transparent and without any crystallographic defects. In addition to that, it indicates that the increasing of adhesive nature of the films at 0.1 molarity with the $InCl_3$ precursor.

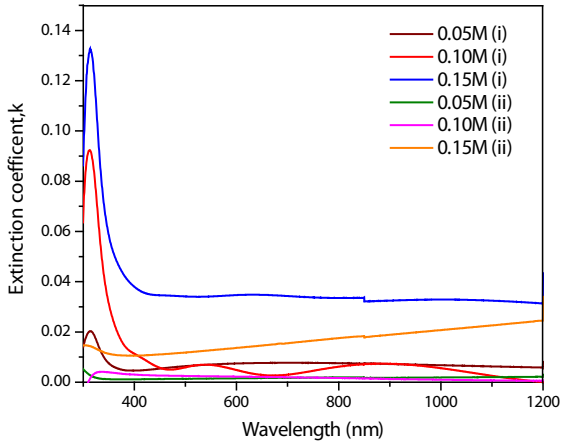


Figure 7: Variation of Extinction Coefficient with Wavelength of In_2O_3 Films at Different Molarities for the Precursors (i) $InCl_3$ and (ii) $InNO_3$

The refractive index (n) of the film can be evaluated using the relation [18]

$$n = \frac{(1+R)^{1/2}}{(1-R)^{1/2}} \quad (8)$$

Where R is the normal reflectance.Fig.8 shows the variation of refractive index with wavelength of the films at different molarities for the precursors (i) $InCl_3$ and (ii) $InNO_3$. In these spectra for $InCl_3$ precursor, the films deposited for 0.05M and 0.1M having maximum refractive index 2.644 and 2.652 for the wavelengths 327nm and 370nm respectively. The 0.15M exhibits different property as the refractive index is minimum in the U-V region and maximum in the visible and near infrared regions. This may be due to the porosity and pinholes in the film surface with randomly oriented grains. For $InNO_3$ precursor the films deposited at 0.15M having maximum refractive index 2.644 for the wavelength 303nm and 0.05M and 0.1M having maximum refractive index 2.137 and 1.934 for the wavelengths 334nm and 302nm respectively. On comparing the precursors the refractive index is maximum at 0.05M and 0.1M rather 0.15M for $InCl_3$ and for $InNO_3$ is vice-versa.

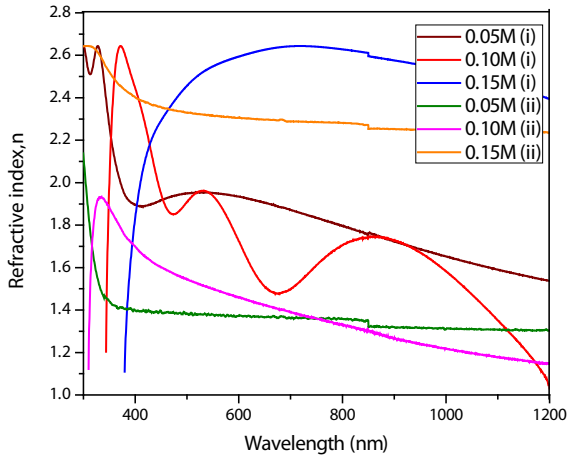


Figure 8: Variation of Refractive Index with Wavelength of In_2O_3 Films at Different Molarities for the Precursors (i) $InCl_3$ and (i) $InNO_3$

The dielectric constant, ε of the films is determined by the relation [19-20]

$$\varepsilon = \varepsilon_1 + \varepsilon_2 = (\varepsilon_1^2 + \varepsilon_2^2)^{1/2} \quad (9)$$

$$\varepsilon_1 = n^2 - k^2 \text{ and } \varepsilon_2 = 2nk \quad (10)$$

where, ε_1 and ε_2 are the real and imaginary parts of the dielectric constant.

The dielectric constant or the absolute complex permittivity of a material depends on temperature, pressure and frequency, etc. The frequency dependence of real and imaginary parts of the dielectric constant for the films at different molarities for the precursors (i) $InCl_3$ and (ii) $InNO_3$ are as shown in fig.9 and fig.10 respectively. From the figures the films at 0.15M for both the precursor exhibit different variation characteristics than the other molarities. The molarities except the film at 0.15M are having maximum value of real and imaginary parts of dielectric constant in the U-V region and minimum in the visible and near infrared regions. Particularly the film at 0.1M for $InCl_3$ is observed to have the higher values of real and imaginary parts of the dielectric constant than the other molarity deposition, and it may be due electronic, atomic and orientation polarization of the material.

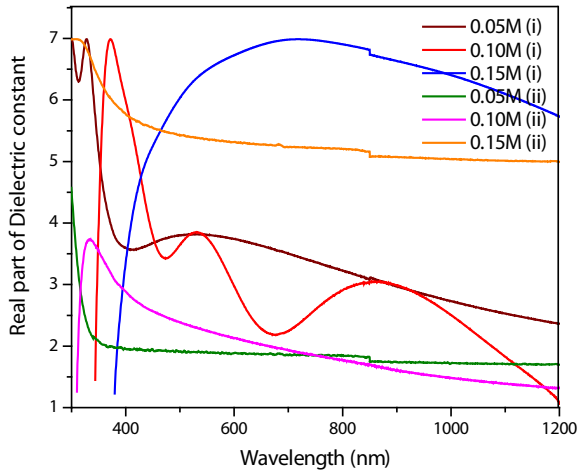


Figure 9: Variation of Real Part of dielectric constant with Wavelength of In_2O_3 Films at Different Molarities for the Precursors (i) $InCl_3$ and (ii) $InNO_3$

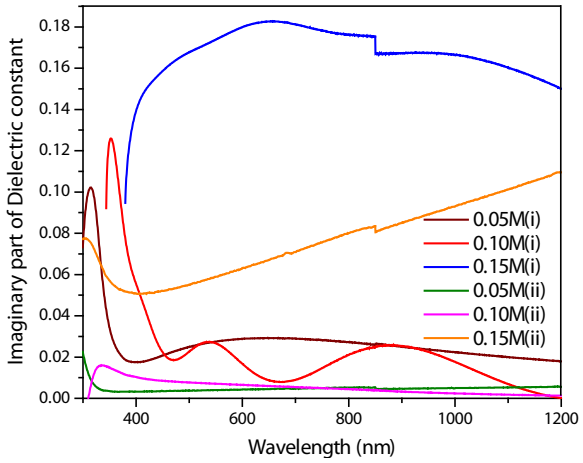


Figure 10: Variation of Imaginary Part of Dielectric Constant with Wavelength of In_2O_3 Films at Different Molarities for the Precursors (i) $InCl_3$ and (ii) $InNO_3$

The photoluminescence spectra of In_2O_3 films were obtained using bombardment of an excitation source with wavelength of 325nm.The fig.11 shows the PL spectra of the films deposited at different molarities for the precursors (i) $InCl_3$ and (ii) $InNO_3$. In the spectra, for all the films, violet emission is observed except the film at 0.15M for $InNO_3$ precursor. It emits indigo light with less PL intensity. For the $InCl_3$ precursor the film at 0.1M alone is having maximum PL intensity. But for the $InNO_3$ precursor the films at all the molarities are having maximum PL intensity. From photoluminescence spectra of various molarities precursors, the intensity of PL emission and also other optical constants are observed to be maximum for

the film at 0.1M with $InCl_3$ precursor, which implies that more radiative recombination occurs with the excitation source of wavelength of 325nm. The observed optical parameters of In_2O_3 films deposited at different molarities and different precursors are listed in Table.2.

Table 2: Optical Parameters of In_2O_3 Films Deposited at Different Molarities for the Precursors (i) $InCl_3$ and (ii) $InNO_3$

Molarity	Band Gap energy(eV)		Refractive index		Extinction coefficient (minimum value)		Dielectric constant, real part		Dielectric constant, imaginary part		PL intensity x106 (a.u)	
	(i)	(ii)	(i)	(ii)	(i)	(ii)	(i)	(ii)	(i)	(ii)	(i)	(ii)
0 .05M	3.647	3.598	2.644	2.137	0.004	0.001	7.002	4.577	0.101	0.023	2.22	6.59
0.1M	3.689	3.133	2.652	1.934	0.002	0.002	7.015	3.765	0.126	0.016	6.45	6.97
0.15M	3.663	3.374	2.648	2.644	0.034	0.010	6.989	6.989	0.182	0.077	0.20	6.952

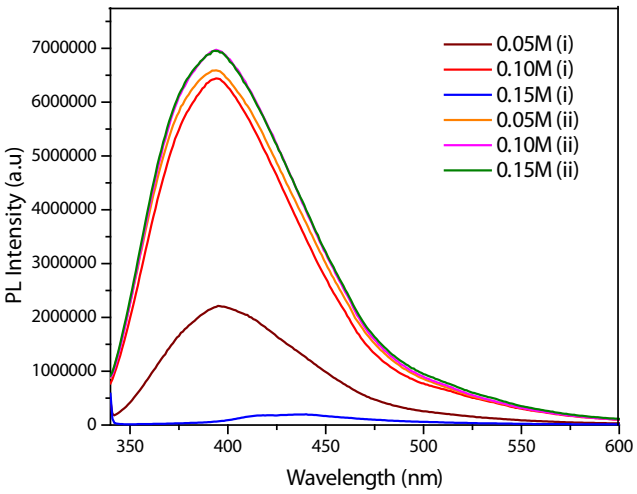


Figure 11: PL Spectra of the Films Deposited at Different Molarities for the Precursors (i) $InCl_3$ and (ii) $InNO_3$

Electrical Properties

The electrical properties are studied for these films prepared at different precursors with optimized molar concentration 0.1M. The hot probe and the Hall Effect measurements have confirmed n-type semiconducting nature of the In_2O_3 films. For the films prepared at $InCl_3$ precursor (0.1M), the carrier density is approximately $3.4x10^{19}cm^{-3}$ with an electrical resistivity of $8.92x10^{-3}$ Ωcm and mobility 80.2 cm2/Vs have been obtained. Moreover, as the film was prepared with Indium nitrate precursor (0.1M), the carrier density 4.26 $x10^{18}$ cm^3 with an electrical resistivity of $1.924x10^{-2}$ Ωcm and mobility -76.8cm^2 /Vs is observed. The resistivity is low for the films prepared at $InCl_3$ that shows the better crystallinity compared with indium nitrate precursor. The Hall Effect result suggested that the In_2O_3 thin films (using InCl3) should be effectively used as optoelectronic application.

Conclusion

In_2O_3 films were deposited by spray pyrolysis using Indium chloride and Indium Nitrate as precursors. The films were deposited at 0.05M, 0.10M and 0.15M. By comparing structural and morphological characteristics, the film deposited at 0.10M for $InCl_3$ precursor has (222) plane as preferred orienting exhibiting improved crystallinity, with maximum grain size and minimum microstrain and dislocation density. The Chlorides are homogeneous anions and Nitrates are heterogeneous anions. So $InCl_3$ is having stronger crystalline structure than $InNO_3$. The optical constants obtained using U-V and PL analysis indicate that the film deposited for 0.10M at 500°C is having band gap energy as 3.689 eV, high refractive index, low extinction coefficient and high intense PL emission. Taking into account that chlorides are more electronegative than nitrates, the nucleation density and deposition rate is higher for the film with $InCl_3$ than $InNO_3$. It could be concluded that structural, morphological and optical characteristics of In_2O_3 films were found to be sensitive to the variation of molarity and precursor, the films with $InCl_3$ as precursor had more advantageous properties than the $InNO_3$. Furthermore, the film deposited at 0.10M with $InCl_3$ shows improved properties, making it suitable for gas sensing and optoelectronic applications.

References

1. Z.M. Jarzebski, Properties of transparent conducting oxide films, Phys. Stat. Sol. (A) 71 (1982)13-41.
2. C.G. Granquist, Electro chromic tungsten oxide films: Review of progress, 1993-1998, Solar energy matter, Solar Cells 60 (2000) 201-262.
3. A.K. Jana, Review of solar cells based on dyes, J. Photochem. Photobiol.A Chem. 132 (2000) 1-17.
4. R.G. Gordon, Criteria for choosing transparent conductors,Mater. Res. Soc. Bull. 25 (2000) 52-57.
5. H. Mexiner, J. Gerblinger, U. Lampe, M. Fleicher, Thin film gas sensors based on semiconducting metal oxides, Sens. Actuators B, B23 (1995) 119-125.
6. E.B. Ali, H.El. Maliki, J.C. Bernede, M. Sahnoun, A. Khelil, O. Saadane, In_2O_3 deposited by reactive evaporation of Indium in Oxygen atmosphere-Influence of post-annealing treatment on optical and electrical properties,Mater. Chem. Phys. 73 (2002) 78-85.
7. D.H. Lowndes, D.B. Geohegan, A.A. Puretzky, D.P. Norton, C.M. Rouleau, Synthesis of novel thin-film materials by pulsed Laser deposition, Science 273 (1996) 898-903.
8. T.L. Barr, Y.L. Liu, An x-ray photo electron spectroscopy study of the valance band structure of Indium oxides, J. Phys. Chem. Solids 50 (1989) 657-664.
9. R.B.H. Tahar, T. Ban, Y. Ohya, Y.Takahashi, Optical, structural and electrical properties of indium oxide thinfilms prepared by the sol-gel method, J. Appl.Phys. 82 (1997) 865-570.
10. J. Kane, H.P. Schweizer, W.Kein, Chemical vapour deposition of transparent electrically conducting layers of Indium Oxide doped with Tin, Thin Solid Films 29 (1975) 155-163.
11. J.C. Manifacier, L. Szepessy, J.F. Bresse, M. Peroten, R.Stuck, In_2O_3:(Sn) and SnO_2:(F) films- Application to solar energy conversion: part 1-preparation and characterization, Mater. Res. Bull. 14 (1979) 109-119.
12. J. Joseph Prince, S. Ramamurthy, B. Subramanian, C. Sanjeeviraja, M. Jayachandran, Spray pyrolysis growth and material properties of In_2O_3 films, Journal of Crystal Growth 240 (2002)142-151.
13. M.Jothibas, C.Manoharan, S.Ramalingam, S.Dhanapandian, S.Johnson Jeyakumar, M. Bououdina, preparation, characterization, spectroscopic (FT-IR, FT-Raman, UV and visible) studies, optical properties and Kubo gap analysis of In_2O_3 thin films, Journal of Molecular Structure 1049 (2013) 239–249.
14. K.L. Chopra, S. Major, D.K. Pandya, Transparent conductors-A status review, Thin Solid Films 102 (1983) 1-46.
15. A.L. Fahrenbruch, R.H. Bube (Eds.), Fundamentals of Solar Cells, Academic, New York, 1993.
16. K.L. Chopra, S.R. Das, Thin Film Solar Cells, Plenum Press, New York,1983.
17. M.Jothibas, C.Manoharan, S.Ramalingam, S.Dhanapandian, M.Bououdina, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 122 (2014) 171-178.
18. D. Gielo, M.M. Miccocci, R. Rella, P.Siciano and A.Tepore, Optical absorption and photo conductivity in amorphous Indium selenide thin films, Thin Solid Films, 148 (1987) 273-278.
19. F. Yakuphanoglu, S. Ilican, M.Caglar and Y. Caclar, The determination of the optical band and optical constants of non-crystalline and crystalline ZnO thinfilms deposited by spray pyrolysis, J.Optoelect.Adv.Mater., 9 (2007) 2180-2185.
20. M.Jothibas, C.Manoharan, S.Dhanapandian and S.Johnson Jeyakumar, Influence of Precursor Concentration on Sprayed In_2O_3Thin Films, Asian Journal of Chemistry; Vol. 25, Supplementary Issue (2013),S59-S64.

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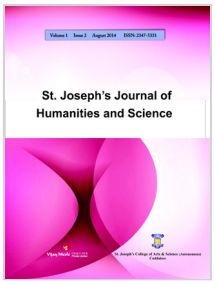

Crystal Growth, Optical and Micro Hardness Studies of an Organic Nonlinear Optical PNDG Single Crystal

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- Dr. A. Christy Ferdinand[*]
- V. Manikandan[**]
- S. Sornambal[***]

Abstract

Transparent single crystals of PNDG were grown by slow evaporation solution technique to confirm the crystal structure. The grown crystals were subjected to single crystal and it has been studied the structural bands using FTIR spectrum in the region 400-4000cm^{-1}. Optical transmittance of PNDG single crystal has been measured by UV-visible transmittance spectrum. The mechanical strength and work hardening for PNDG crystal is studied using Vicker's micro hardness method and the elastic stiffness is calculated using Wooster's empirical formula.

Keywords: Glycine, β-naphthol, PNDG, UV-Vis Spectrometry, FTIR, Vicker's Microhardness.

Introduction

Non linear optics is a frontier field in science and technology which has found wide applications in the field of telecommunication, optical information, optical storage device etc.,[1&2]. The NLO properties of large organic molecules have been the subject of extensive theoretical and experimental investigations. Among organic crystals for NLO applications, amino acids display specific features of interest such as (i) molecular chirality, which secures acentric crystallographic structure, (ii) absence of strongly conjugated bonds, leading to wide transparency ranges in the visible and UV spectral regions, (iii) zwitterionic nature of the molecule, which favors crystal hardness [3-5]. Glycine is the simplest of all amino acids and is known to crystallize in three different polymorphs: α, β, and γ [6,7]. In the present study we have reported about the growth aspects of PNDG single crystals by slow evaporation method. Here the glycine transforms into α-phase on heating. The α-glycine has the space group. In the solid state,α-glycine contains a deprotonated carboxylic acid group(COO^-) and protonated amino acid group(NH_3^+). This dipolar nature combined with centrosymmetric point group makes PNDG an ideal candidate for NLO application. The grown crystals have been subjected into FTIR, UV-Visible and Micro Hardness studies.

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Experimental Procedure

The saturated solution was prepared using commercially available glycine (CH2 NH2 COOH) and β-naphthol. Glycine and β-naphthol was dissolved in a 100 ml beaker using water and dmso as the solvent. The solution was stirred well for about six hours at room temperature and the saturated solution was filtered with Whatman (Grade No.1) filter paper in clean vessel. The vessels containing the solutions were covered with perforated polythene sheets and kept at dust free atmosphere. The solution was allowed for slow evaporation. Crystals with (1.1 mm * 0.8 mm) was harvested and then subjected to characterization studies.

Results and Discussion

FTIR Spectral Analysis

The infrared spectroscopy is effectively used to identify the functional groups of the samples. Fourier transform infrared (FTIR) was recorded in the range 400-4000cm^{-1} using the Perkin Elmer grating infrared spectrophotometer. The recorded Fourier transform infra-red (FT-IR) spectrum of PNDG crystal is shown in Figure 1.

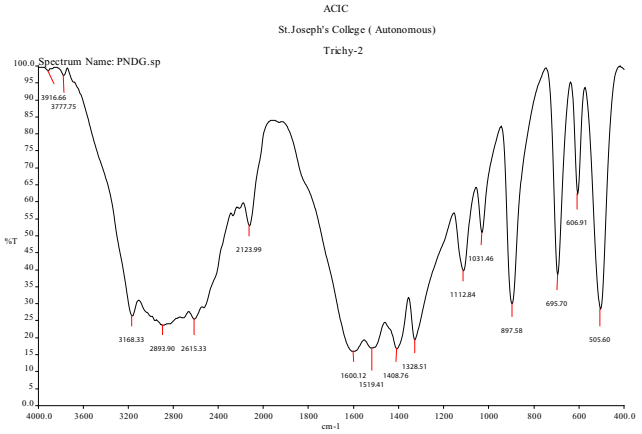

Figure 1: FTIR Spectrum of PNDG Crystal

In the FT-IR spectrum the peak observed at 3168 cm^{-1} are assigned to NH_3^+ stretching vibration. The peak observed at 2893cm^{-1} is attributed to C-H group. The peak observed at 2615cm^{-1} is contributed to NH_3^+ stretching vibration. The combinational bond observed from the spectrum is very strong (2123 cm^{-1}) compared to α-glycine (2121 cm^{-1}). The peak observed at 1600cm^{-1} is due to asymmetric CO_2 stretching. The peak observed at 1519cm^{-1} is assigned to NH_3^+. The peak observed at 1408 cm^{-1} correspond to COO^- symmetric stretching. The peak observed at 1328cm^{-1} are attributed to CH_2 twisting. The peak observed at 1112cm^{-1} is due to NH_3^+rocking.The peak observed at 1031cm^{-1}are assigned to CCN asymmetric stretching vibration. The peak observed at 897cm^{-1} is contributed to CCN symmetric stretching vibration. The peak observed at 695cm^{-1} corresponds to COO^- bending. The peak observed at 606cm^{-1} is due to COO^- wagging. The peak observed at 505 cm^{-1} is assigned to COO^- rocking.

It is concluded that from the FTIR data comparison, the observed functional group of the grown PNDG single crystal are in good agreement with the literature value [8] of α-Glycine and they are presented in the table 1.

Table 1: Comparison of FTIR Spectrum of PNDG Crystal with α-Glycine

PURE GLYCINE	PNDG	α- GLYCINE (Literature value)	TENTATIVE ASSIGNMENT
893	897(S)	898	ν_s (CCN)
910	1031(VS)	1030	ν_s (CCN)
1033	1112(S)	1109	$\rho(NH_3^+)$
1133	1328(S)	1328	$\tau(CH_2)$
1333	1408(M)	1409	ν_s (COO^-)
1413	1519(W)	1513	(NH_3^+)
-	1600(W)	1609	ν_{as} (CO_2)
-	2123(S)	2121	Combinational Bond
-	3168(S)	3169	$\nu(NH_3^+)$
-			

τ – Twisting , ρ – Rocking , δ – Bending , ω – Wagging, – Stretching, S - Strong , VS – Very Strong , W – Weak, M – Medium

UV-Visible Spectral Analysis

The UV-Vis spectrum gives limited information about the structure of the molecule because the absorption of UV and visible light involves promotion of the electrons in the σ and π orbital from the ground state to a higher energy state. To find the transmission range optical transmission spectrum of the PNDG was recorded. The recorded transmission and absorption spectra are shown in the figure 2&3. The transmission was found at 318nm and the absorption SPR peak was found at 192nm. The crystal is found to be transparent in the visible and near

IR region,an essential parameter required for frequency doubling process[9]. This is the advantage of the use of amino acids where the absence of strongly conjugated bonds leads to the wider transparency ranges in the visible and UV spectral regions[10]. The lower cut off at 200nm combined with the very good transparency window makes the material suitable for optoelectronic applications.

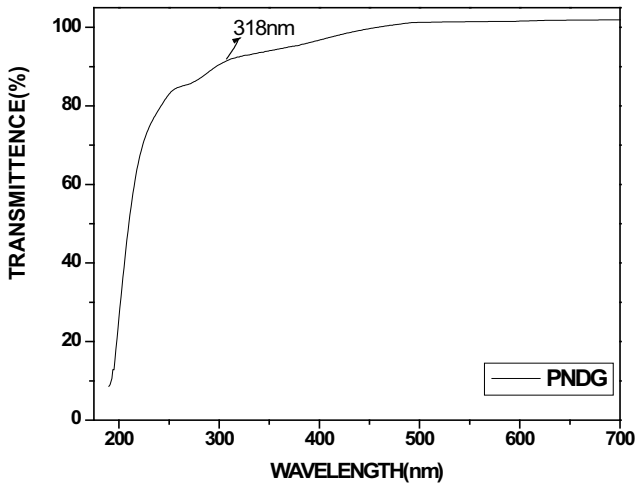

Figure 2: UV-Vis Transmittance Spectrum of PNDG Crystal

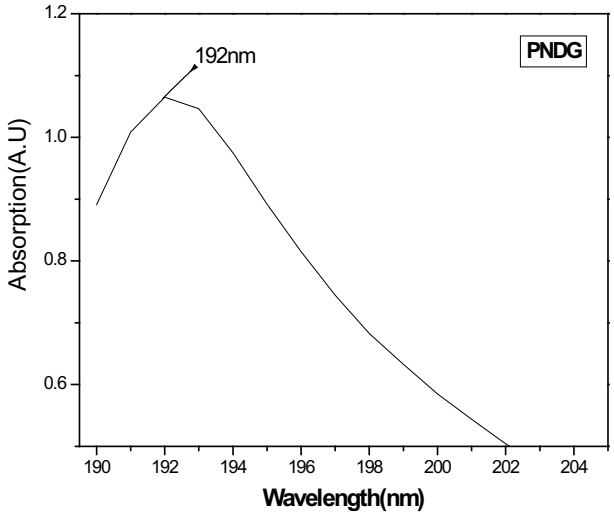

Figure 3: UV-Vis Absorption Spectrum of PNDG Crystal

Micro Hardness Analysis

The hardness of a material is a measure of its resistance to plastic deformation. Microhardness studies are carried out using MHT-10 microhardness tester (Anton-Paar) for PNDG crystals to determine its hardness. Load of different magnitudes as 25gm, 50 gm, 100 gm were applied. The indentation time was fixed as 10 s for each trial. Repeated trials were performed to ascertain the correctness of the observed results.

The Vickers microhardness number (H_V) was calculated using the equation [11,12] given as follows:

$$H_V = 1.8544\ P/d^2\ (kg/mm^2) \quad (1)$$

Where P is the indenter load (kg) and d is the diagonal length of the impression (mm) and 1.8544 is a constant of a geometrical factor for the diamond pyramid. Figure 3 shows that the hardness of the grown PNDG single crystal increases with increase in load. Using Meyers law we calculate the Meyer's index (n) to analyse the nature of the material. The size of intentation and load are related through Meyer's law[13-15],

$$P = k_1 d^n \quad (2)$$

From the slope of log P vs log d shown in figure 4 gives the estimated n value. In the present study the obtained n value of PNDG crystal is 3.6 and we find that the material belongs to the soft material category. Since the value of n is larger than 2, the hardness of the material increases with increase of load conforming the prediction of Onitsch[16].According to Hays-Kendall's approach load dependent hardness may be expressed by,

$$P = W + A_1 d^2 \quad (3)$$

$$H_0 = 1854\ A_1 \quad (4)$$

Where W is the minimum load initiate plastic deformation.A_1 is the load independent constant,H_0 is the corrected hardness. The value of W and A_1 can be calculated by plotting the graph between P and d^2. The estimated value of W and A_1 from the plot drawn between P and d^2 is shown in the figure 5. The value of W and H_0 for various loads are given in the table 5.3. Also the elastic stiffness constant is calculated using Wooster's empirical formula [17], which is given by

$$C_{11} = (Hv)^{7/4} \quad (5)$$

The Hardness Parametrs of PNDG crystal for various loads is also given in table 2.

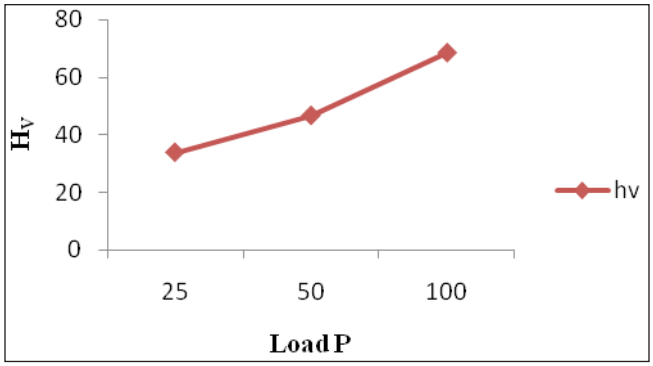

Figure 4: Graph Between Applied Load ρ and Vickers Micro Hardness Number

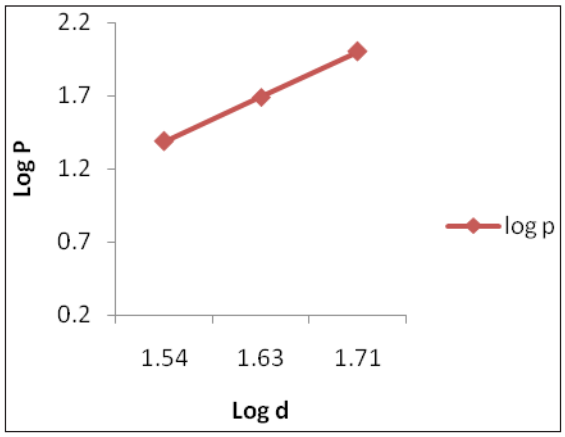

Figure 5: Graph Between Log d and Log ρ

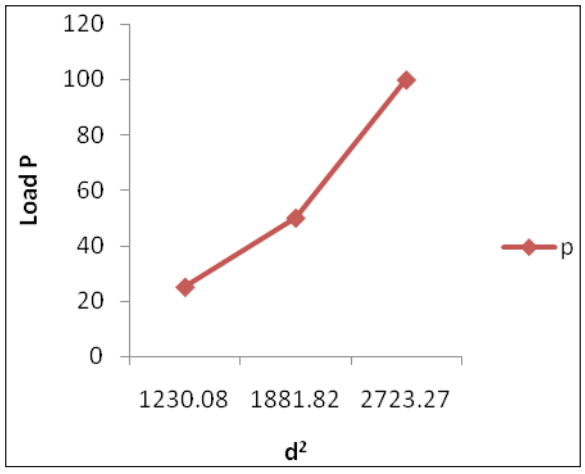

Figure 6: Graph Between d^2 and Applied Load ρ

Table 2: Hardness Parameters of PNDG Crystal

Load(P)	N	H_V	A_1	W	H_0	$C_{11}*10^{14}$pa
25	3.6	35.75	0.05	-36.504	92.72	5.2267
50	3.6	46.55	0.05	-44.091	92.72	8.2958
100	3.6	68.35	0.05	-36.164	92.72	16.2477

Conclusion

Good quality transparent single crystals of PNDG have been grown by slow evaporation technique at room temperature. From the FTIR spectrum ,the observed functional group of the grown PNDG single crystal are in good agreement with the literature value of α-glycine and a very strong bond is observed at 1031cm^{-1} due to symmetric CNN stretching. UV-Vis spectra shows that the grown PNDG single crystal has a good transmission window in the visible region suitable for NLO application and the lower cut of frequency wavelength is192 nm. Vickers Microhardness study on the PNDG single crystal reveals that the H_V and C_{11} increases with increase in load.

Reference

1. N. Vijayan, R. RameshBabu, M. Gunasekaran, R. Gopalakrishnan, R. Kumaresan, P. Ramasamy, C. N. Lan, J. Cryst. Growth, 275 (2005), pp. 1935.
2. C. Krishnan, P. Selvarajan, T. H. Freeda, Material Letters,62(2008), pp. 4414.
3. M. D. Aggarwal, J. Stephens, A. K. Batra, and R. B. Lal, J. Optoelectronics Adv Mater, vol. 5, (2003), pp. 555.
4. C. Razzetti, M. Ardoino, L. Zanotti, M. Zha, and C. Paorici, Cryst.Research Technol, vol. 37, May(2002), pp. 456-465.
5. M.Hanneman, Metall, Manchu 23(1941), pp.135.
6. G. He. V. Bhamidi, S. R Wilson, R. B. H Tan, J. A Paul, C. F Kenis, Zukoski, Crystal Growth, Des.6(2006) , pp. 1746-1749.
7. N. Doki, M. Yokota, K. Kido, S. Sasaki, N. Kubota, Cryst. Growth Des.4 (2004), pp. 103-107.
8. S. Anbu Chudar Azhagan , S. Ganesan, Arabian Journal of Chemistry (2013).
9. C. N. R. Rao, Ultraviolet and visible spectroscopy of organic compounds, Prentice Hall Pvt. Ltd., New Delhi (1984), pp.60-64.
10. C. Razzetti, M. Ardoino, L. Zanotti, M. Zha, M. Parorici, cryst. Res. Technol. 37 (2002), pp.456.

11. S. Suresh, A. Ramanand, D. Jayaraman, Optoelectron. Adv. Mater. Rapid Commun. 4 (2010), pp. 1987-1989.
12. S. S. Raman and A. M. P, Kaliyamurthyanand, J. Optoelectronics and Biomedical Materials, vol. 1,July (2010), pp. 129-139.
13. B.Lal , K.K.Bamzi , P.N.Kotru , B.M.Wanklyn, Mater. Chem. Phys .85 (2004), pp.353-365.
14. V. Gupta, K. K. Bamzi, P. N. Kotru, B. M. Wanklyn, Mater. Chem. Phys. 89 (2005), pp.64-71.
15. S. Dhanuskodi, T. C. Sabari Girisun, G. Bhagavanbarayanan, S. Uma, J. Philip, Mater. Chem. Phys.126 (2011), pp.463-469.
16. E. M. Onitsch, Mikroscopia 2 (1947), pp.131.
17. S. Karan, S. P. S Gupta, Mater. Sci. Eng. A 398 (2005), pp.198-203.
18. R. Parimaladevi, C. Sekar, Spectrochemica acta, Part A,76 (2010), pp.490-495.
19. Neelam Rani, N. Vijayan, M. A Wahab, G. Bhagavannarayana, B. Riscob, K. K Naurya, Optik-Int. J. Light Electron Opt (2012).

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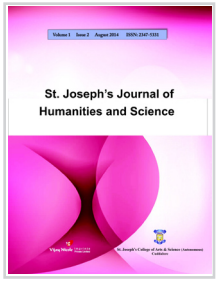

Efficiency of Cart and Regression Trees in Predicting Student's Absenteeism in an Academic Year

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Abstract

Educational data mining is being used to study the data available in the educational field and bring out the hidden knowledge from it. Classification methods like decision trees, rule mining can be applied on the educational data for predicting the students behavior. This paper focuses on the reason for the leave taken by the student in an academic year. The first step of the study is to gather student's data by using a questionnaire. We collected data from 123 students who were under graduates from a private college which is situated in a semi-rural area. The second step is to clean the data which is appropriate for mining purpose and choose the relevant attributes and the classification is done using the gender attribute. Decision tree was constructed using CART Algorithm by using the Gini index as the splitting criterion. This knowledge is used to identify the reason for the leave taken by the student and help to improve the quality of the environment and also to improve the performance of the student.

Keywords: Data Mining, Decision Trees, CART, Regression Trees.

Introduction

Currently many educational institutions, especially small-medium educational institutions are facing problems with the lack of attendance among the students. The universities will allow the students to write the semester if they have attendance above 80%, student having attendance percentage below 80% will lack attendance and are not permitted to write the semester exam. All educational institutions are facing this problem and so this research aims to find the reason for students absence in the college and take immediate actions to overcome this problem.

Literature Survey

Catherine Butchart, Firat Ismailoglu, presented their paper in 2012 in that, they studied about the increasing number of oldest old people in the future. They identify the potential predictors of inpatient mortality in patients

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over 90 years old admitted acutely to the hospital due to various medical emergencies in two UK centers[1].

Chong Yau Fu presented his paper in combining loglinear model with CART in application to birth data in 2003. In that CART method is based on variation (impurity) reduction for binary splitting; a tree structure was produced as a result of the splitting process[2].

Sunita B. Aher and Lobo, L.M.R.J. presented their paper on the comparison of the five classification algorithm to choose the best classification algorithm for Course Recommendation system. These five classification algorithms are ADTree, Simple Cart, J48, ZeroR & Naive Bays Classification Algorithm. They compare these six algorithms using open source data mining tool Weka & present the result.

F. Questier, R. Put presented their paper on CART approaches for both supervised and unsupervised feature selection in 2004. They describe feature selection by modelling one response variable (y) by some explanatory variable (x).

Background Knowledge

Databases are rich with hidden information that can be used for intelligent decision making. Classification and prediction are two forms of data analysis that are used to extract models describing important data classes or to predict future data trends. Such analysis can help provide us with a better understanding of the data at large. Classification and prediction have numerous applications, including fraud detection, target marketing, performance prediction, manufacturing and medical diagnosis. Classification is used to find the class label for the data and prediction is used find the value in the class label[5]

Classification By Decision Tree Induction

Decision tree induction is the learning of decision trees from class-labeled training tuples. A decision tree is a flow chart tree structure, in which each internal node (non-leaf node) denotes a test on an attribute, each branch represents an outcome of the test, and each leaf node (or terminal node) holds a class label. The topmost node in a tree is the root node[6].

Decision Tree Induction Algorithm

During the late 1970s and early 1980s J.Ross Quinlan a researcher in machine learning developed a decision tree algorithm known as ID3(Iterative Dichotomiser). ID3 adopt a greedy (i.e. nonbacktracking) approach in which decision trees are constructed in a top-down recursive divide-and-conquer manner. Most algorithms for decision tree induction also follow such a top-down approach, which starts with a training set of tuples and their associated class labels. The training set is recursively partitioned into smaller subsets as the tree is being built[7]. A basic decision tree algorithm is summarized below.

Algorithm: Generate Decision Tree

Generate a decision tree from the training tuples of data partition D.

Input:

- Data partition, D, which is a set of training tuples and their associated class lables.
- Attribute_list, the set of candidate attributes.
- Attribute_selection_method, a procedure to determine the splitting criterion that "best" partitions the data tuples into individual classes. This criterion consists of a splitting_ attribute and possibly either a split point or splitting subset.

Output: A decision tree

Method:

1. Create a node N:
2. If tuples in D are all of the same class C,
3. Return N as a leaf node labeled with the class C
4. If attribute_list is empty then
5. Return N as a leaf node labeled with the majority class in D;//majority voting
6. Apply Attribute_selection_method (D, attribute_list) to find the "best" splitting_ criterion";
7. Label node N with splitting_criterion;
8. If splitting_attribute is discrete-valued and multiway splits allowed then//not restricted to binary trees
9. Attribute_list→attribute_list-splitting attribute;//remove splitting_attribute

10. For each outcome j of splitting_criterion // partition the tuples and grow subtrees for each partition.
11. Let Dj be the set of data tuples in D satisfying outcome j;//a partition
12. If Dj is empty then
13. Attach a leaf labeled with the majority class in D to node N;
14. Else attach the node returned by Generate_ decision_tree(Dj,attribute_list)to node N; endfor
15. Return N;

Classification and Regression Tree (Cart)

Classification and Regression Trees (CART) was introduced by Breiman et al. It is a statistical technique that can select from a large number of explanatory variables(x) those that are most important in determining the response variable (y) to be explained. The CART steps can be summarized as follows[8].

1. Assign all objects to root node.
2. Split each explanatory variable at all its possible split points (that it is in between all the values observed for that variable in the considered node.)
3. For each split point, split the parent node into two child nodes by separating the objects with values lower and higher than the split point for the considered explanatory variable.
4. Select the variable and split point with the highest reduction of impurity.
5. Perform the split of the parent node into two child nodes according to the selected split point.
6. Repeat steps 2-5, using each node as a new parent node, until the tree has maximum size.
7. Prune the tree back using cross-validation to select the optimal sized tree.

For regression trees with numerical response variable the impurity calculated at step 4 can be defined as the total sum of squares of the response values around the mean of each node. For a node with n objects the impurity is then defined as:

Impurity = $\sum_{i=1}^{n}(yi - \bar{y})^2$

For classification trees with a categorical response variable the impurity is defined with i.e. the Gini index of diversity. The Gini index of a node with n objects and c possible classes is defined as:

Gini = 1- $\sum_{j=1}^{c}\left(\frac{nj}{n}\right)^2$

Where n_j is the number of objects from class j present in the node.

Data Collection

The data are collected from a private college at Ulundurpet in Villupuram district. There were 123 records collected from the students who are doing under graduate course who belong to the age group 18 to 23. Among the 123 students 85 were male and 38 were female candidates. The data are stored in Microsoft Excel 2010. A questionnaire was prepared and given to the students of the department of BCA, BBA, BCOM. The questionnaire contains 30 questions and five point scale was used. The analysis is done by using the gender attribute.

The data used for data mining contains 123 records and have 30 dimensional attribute namely name, gender, age, department, year, mode of transport, college location, home location, test, cinema, festival, sick, miss bus, friend leave, subject boring, staff question, exam study, result, occasionally, institution work, part time job, assignment, pay fees, native, accident, dress code, commitment friends, college care, impress, problem in college. For our study name is not necessary; so we omitted the attribute and took the 29 attribute for classification.

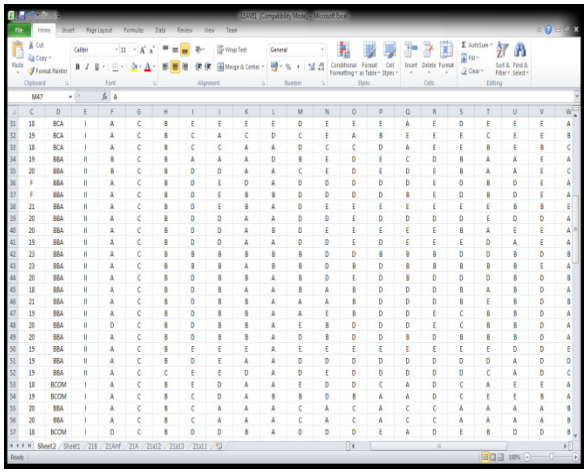


Figure 1: Data Used for Mining

System Framework

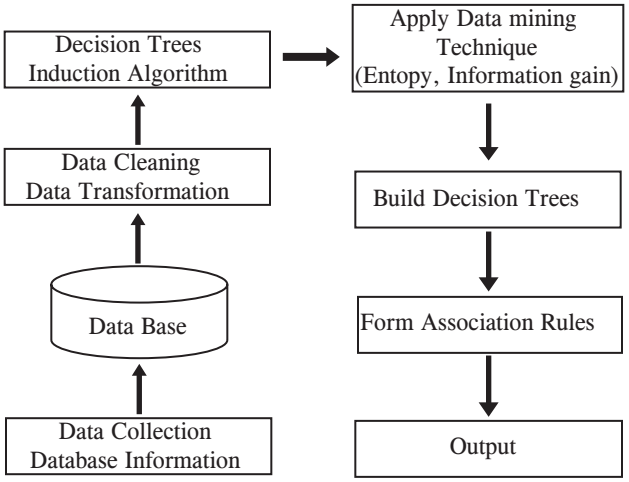


Figure 2: System Frame Work

Experimental Setup

Tanagra is a open source software used for data mining. It supports all the basic type of data formats like *.xls, *.txt etc. and it is very user friendly. The data set is implemented in Tanagra by the following method.

- Open the Tanagra software and go to the file menu and click open then insert the data you want to evaluate.
- Go to Data Visualization and select view data set and drag in to the data set.
- Select the view data set and right click and click execute and then click view then the data is displayed on the right side screen.
- Drag the Define status from the icon and give the target attribute as gender and in input select all the attributes.
- Go to spv learning and select C-RT and drag into the Define status and right click it and click execute and then click view; then the results are displayed in the right side screen.

Evaluation

The analysis of the data is done on the basis of gender i.e. the reason why a male student takes leave and the reason why a female student takes leave from the college by applying Entropy and Information gain

Table 1: Total Records

MALE	FEMALE	TOTAL
85	38	123

$$\text{Gini} = 1 - \sum_{j=1}^{c} \left(\frac{nj}{n}\right)^2$$

$$\text{Gini (D)} = 1 - \left(\frac{85}{123}\right)^2 - \left(\frac{38}{123}\right)^2 = 0.428$$

Table 2: Total records for the attribute Job

JOB	MALE	FEMALE	TOTAL
Strong agree	25	1	26
Agree	28	2	30
Neutral	6	8	14
Disagree	14	13	27
Strong Disagree	12	14	26
TOTAL	**85**	**38**	**123**

The Gini for the attribute part time job is

$$= \left(\frac{26}{123}\right)\left[1 - \left(\frac{25}{26}\right)^2 - \left(\frac{1}{26}\right)^2\right] +$$

$$\left(\frac{30}{123}\right)\left[1 - \left(\frac{28}{30}\right)^2 - \left(\frac{2}{30}\right)^2\right] +$$

$$\left(\frac{14}{123}\right)\left[1 - \left(\frac{6}{14}\right)^2 - \left(\frac{8}{14}\right)^2\right] +$$

$$\left(\frac{27}{123}\right)\left[1 - \left(\frac{14}{27}\right)^2 - \left(\frac{13}{27}\right)^2\right] +$$

$$\left(\frac{26}{123}\right)\left[1 - \left(\frac{12}{26}\right)^2 - \left(\frac{14}{26}\right)^2\right]$$

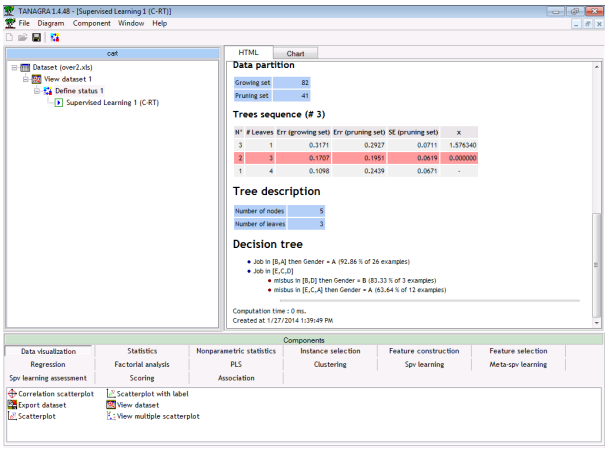
$$= 0.0156 + 0.0302 + 0.0553 + 0.1096 + 0.1050$$
$$= 0.3157$$

$$\text{Gini (job)} = 0.428 - 0.3157$$
$$= 0.1123$$

The information gain for the attribute job has the highest value in the database and the other values in the table are listed below.

The job attribute is taken as the root node of the tree and the 123 records are split by the branches of the job as strongly agree 26 records and Agree 30 records and Neutral 14 records and Disagree 27 records and Strongly Disagree 26 records and the process is applied for the each table and decision tree is formed as below.

Result for Our Data Set



- Job in [B,A] then Gender = **A** (92.86 % of 26 examples)
- Job in [E,C,D]
  - misbus in [B,D] then Gender = **B** (83.33 % of 3 examples)
  - misbus in [E,C,A] then Gender = **A** (63.64 % of 12 examples)

Figure 3: Decision Tree in Tanagra

The results obtained from Tanagra is shown in the figure above. Here job attribute is taken as the root node because it has the highest information gain; so all job is the root node and it has five discrete attributes as its values called A) Strongly Agree, B) Agree, C) Neutral, D) Disagree and E) Strongly Disagree. All the five are the branches of the node job and all the 123 records are split according to the values present in the each node and the process is repeated at each node until the leaf node comes or until there is no root node. Here in Tanagra the root is dark circle and next child node is blank circle using this dots we can identify the nodes in Tanagra.

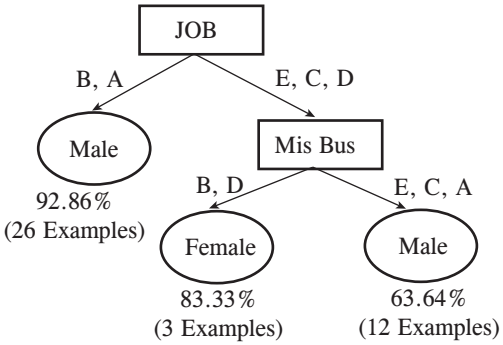


Figure 4: CART Tree for the Job Attribute

The CART Tree for our Dataset obtained from Tanagra is shown in the diagram above. The CART Algorithm used in this model for constructing the CART Tree uses the following parameters such as size before split 10, pruning set size 33%, x-SE rule 1.00, Random generator 1, Show all tree sequence(even if>15) 0.

Discussion

The following are the factors associated with student's absenteeism

- The root node split is considered to indicate the most important single variable, and in this study the job attribute was found to be the factor most strongly linked with student's taking leave.
- The next most important variable related to student's leave is the misbus attribute.

From the total of 123 examples containing 85 male and 38 female the following are the report.

- 92.86% of male students who belong to strongly agree and agree category apply leave to college due to going to job for earning money.
- 83.33% of female apply leave to college when they go to job for earning money and also when they miss the regular bus.
- 63.64% of male apply leave to college when they go to job for earning money and also when they miss the regular bus.

The remaining 27 attributes in the dataset are not considered as much important for the reason of student's absenteeism.

Recommendations

From the above experimental results we know that the job attribute plays a key role on job going students to earn money. To improve good learning environment and the quality of education in the rural and semi-rural areas, our suggestion is that change the college timings such as morning and evening sessions to avoid the students absenteeism for the classes. It was found that students apply leave due to the purpose of studying for the examinations; so if we grant enough study holiday, we can avoid students applying leave to college.

Conclusion

This research aims to study the pattern of students who put leave to the college frequently and the reason

behind the students to apply leave. In this research, the decision tree techniques have been used because it is easy to interpret and contributing to the improved results to be compacted. The smaller models are easier to use and general users can understand more easily. We can obtain the best results in predicting the students' behaviour using Classification and Regression Trees (CART) algorithm.

References

1. Catherine Butchart, Firat Ismailoglu, "Identitficaation of possible determinants of inpatient mortality using classification and RegressionTree(CART)analysisinhospitalized oldest old patients",ELSEVIER,2012,
2. Chong Yau Fu, "Combining loglinear model with classification and regression tree(CART):an application to birth data", ELSEIVER, 2003.
3. Sunita B. Aher and Lobo L.M.R.J." Comparative Study of Classification Algorithms", International Journal of Information Technology and Knowledge Management July-December 2012, Volume 5, No. 2, pp. 239-243.
4. F. Questier, R. Put, "The use of CART and multivariate regression trees for supervised and unsupervised feature selection", ELSEVIER, 2004.
5. Michelian kumber and Jai weihan,"Data Mining Concepts and Techniques".
6. S.Anupama Kumar, Dr.Vijayalakshmi M.N, "Efficiency of Decision Trees in Predicting Students Academic Performance", D.C. Wyld,et al. (Eds):CCSEA 2011.
7. Sunitha B.Aher, Lobo L.M.R.J "Comparitive study of Classification Algorithms", International journal of Information Technology and Knowledge Management, 2012.
8. F. Questier, R. Put, D. Coomans "The use of CART and multivariate regression trees for supervised and unsupervised feature selection", ELSEVIER. 2004.

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Categorical Analysis of Routing Protocols

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Abstract

Increased potential in the use of wireless sensor networks in many applications as disaster management, border protection etc., In recent advances wireless sensor networks have let too many new protocols and it has been especially designed for sensor networks and where energy efficient is considered essential. However most of the attention has been given on routing protocols they might differ according to the application and network architecture. The survey is about recent routing protocols with main categories explored are data-centric, hierarchical and location-based. The routing protocols are mainly responsible for maintaining the routes in network and to ensure reliability. Therefore it is a survey of routing protocols for wireless sensor network with energy efficiency.

Keywords: Wireless sensor networks, routing protocols, classification of protocols, energy-efficient.

I. Introduction

Wireless sensor network has been considered as one of the most important technologies for twenty first century. Nowadays it has received tremendous attention in both all over the world. A wireless sensor network typically consists of a large number of low-cost, low-power, wireless communication and computation capabilities [1-2].

These sensor nodes communicate and accomplish a common task. For example, environment monitoring, industrial process [3].

Sensor nodes are battery-powered and also considered to be energy efficient and expected to operate without any loss and relatively work for long period of time. Thus the unique characteristics present in wireless sensor network provide many new challenges. Routing in sensor network is considered

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to be challenging due to the characteristics present in them. Almost all of the routing protocols can be given as data-centric, hierarchical or location-based and few distinct ones also based on the QOS.The basic philosophy that has been behind wireless sensor network is that, when the capability of each and every sensor node has been limited, the aggregate power of the whole network is been sufficient for the particular required mission.

In wireless sensor network applications the deployment of the sensor nodes has been considered in an ad-hoc fashion without any careful planning and organizing. And once when it is deployed, the sensor nodes must be able to autonomously organize themselves in a wireless communication network.

Due to the severe energy constraint of large number of densely deployed sensor nodes it requires to have a suite of network protocols to implement various network control and to manage functions such as synchronization, node localization and network security.

A large number of research activities have been carried out to explore and overcome the constraint of wireless sensor network and to solve and design with its application and issues.

This paper is organized as follows. In the balance of this section 2, we will briefly summarize the system architecture design issues for sensor network and the implementation in data routing. In section 3, network design objectives. In section 4, network design challenges and its routing issues. In section 5, hierarchical based protocols and their approaches are covered. In section 6, summarizes location based protocols in sensor network. In section 7, data centric protocols are discussed. . In section 8, we describe quality of service (QOS) based protocol. Finally, section 9 concludes with a survey of routing protocols in wireless sensor networks.

II. System Architecture and Design Issues

Depending on the application, the architecture and the design goals also have been considered with the sensor network. Since the routing protocols are been closely related with the system architectural model, we highlight the implication.

A. Network Dynamics

There are three main components in a sensor network. They are the *sensor nodes, sink and monitored event*. Routing messages from or to moving nodes is more challenging since route stability becomes an important optimization factor with energy and bandwidth [5].

B. Node Deployment

Another consideration is the deployment of nodes. It is an application dependent and also it affects the routing protocol. The deployment is either *deterministic or self-organizing*. In deterministic situation the sensors have been placed manually. Whereas in self-organizing the sensor nodes have been scattered randomly.

C. Energy Consideration

In creating an infrastructure, the process of setting up the routes is influenced only by the energy consideration. Most of the time sensors are scattered randomly, over an area of interest and it becomes unavoidable.

D. Data Delivery Models

Depending on the application of the sensor network, the data delivery model can be *continuous event-driven, query-driven and hybrid*. In continuous delivery model each sensor takes place periodically. In event-driven and query-driven models, the transmission of data is triggered and finally in hybrid models it uses a combination of both continuous and event-driven.

E. Node Capabilities

In a sensor network much functionality can be associated with sensor nodes and all the sensor nodes are assumed to be with terms as computations, communication and power. By encaging the three functionalities together at the same time on a node there might be a loss and drain in the energy of the node. Therefore by a heterogeneous environment routing becomes more challenging even.

F. Data Aggregation/Fusion

Data aggregation is a combination of data from different sources by using function such as suppression (eliminating duplicates), min, max and average. Data aggregation technique has been used to achieve energy efficiency and data transfer optimization in a number of routing protocols.

III. Network Design Objectives

Most sensor network is application specific and has different requirements. Thus the main objectives in design of sensor network are as follows:

A. Small Node Size

This small node size will reduce the power and consumption with cost of sensor nodes.

B. Low Node Cost

The sensor nodes have been usually used large in numbers and so it cannot be reused, and in reduction of cost and totally it will result in cost reduction.

C. Low Power Consumption

Since all the sensor networks are powered by battery it becomes often difficult or impossible to consumption with the batteries. So that the lifetime of sensor nodes as the whole network is prolonged.

D. Scalability

Since the sensor nodes in sensor network are been ordered as tens, hundreds, thousands it should be given with a scalable unit according to the different network sizes.

E. Reliability

The network protocols present in the sensor network should provide an error control with a correction mechanisms to ensure the reliability over-noisy, error-prone and time-varying wireless channels.

F. Self-Configurability

In sensor networks the sensor nodes should be able to organize themselves in the communication in the event of topology and failure of nodes.

G. Adaptability

In sensor networks any node may be suddenly failed, joined or moved which may result in changes in node density and network topology. Thus the network protocols designed for sensor network must be adaptive to such density and changes.

H. Channel Utilization

Since sensor networks have limited bandwidth resources, communication protocols designed for sensor networks must be efficiently used to improve channel utilization.

I. Fault Tolerance

Sensor networks are fault tolerant and have the ability of self-testing, self-calibrating and self-repairing.

J. Security

Sensor networks introduce effective security mechanisms to prevent the data information in the network or a sensor node from any other unauthorized access or malicious attacks.

K. *QOS support*

In sensor networks, different applications may have different quality of service requirements in terms of delivery latency and packet loss.

IV. Network Design Challenges and Routing Issues

The design challenges in sensor networks involve in the following main aspects [7]

A. Limited Energy Capacity

Since the sensor nodes are been battery powered, they have limited energy capacity. Thus the routing protocols designed for sensors which should be as energy efficient and thus prolongs the network lifetime.

B. Sensor Locations

Another important challenge that has been found in the routing protocols is by managing the location of sensors.

C. Limited Hardware Resources

This hardware presents many challenges in design for sensor networks which must be considered not only the energy constraint but also the storage capacities in sensor nodes.

D. Massive and Random Node Deployment

Sensor node deployment in wireless sensor networks has been application dependent (i.e.); it can be either manual or random which affects the performance in routing protocol.

E. Network Characteristics and Unreliable Environment

A sensor network generally works on the dynamic and its unreliable environment. Therefore the routing paths must be considered with limited energy and sensor mobility and also increasing in size with coverage and connectivity.

F. Data Aggregation

This data aggregation technique has been used to achieve the energy with efficiency and data transfer optimization in a number of routing protocols.

G. Diverse Sensing Application Requirements

The sensor network has a wide range in diverse applications. Therefore the routing protocols guarantee its accuracy about the physical phenomenon on time.

H. Scalability

The routing protocol must be able to scale network size. Hence the communication links between sensors must be symmetric.

V. Hierarchical Based Protocols

Many research projects have explored hierarchical clustering in wireless sensor network from different aspects [1]. Clustering is energy-efficient communication protocol that has been used by sensors to sensor the data.

In this section we give an example of layered protocols in which an network has been composed of several clumps (or clusters) of sensors. Each clump has been managed by a special node called as cluster head, that has been responsible for all the data transmission.

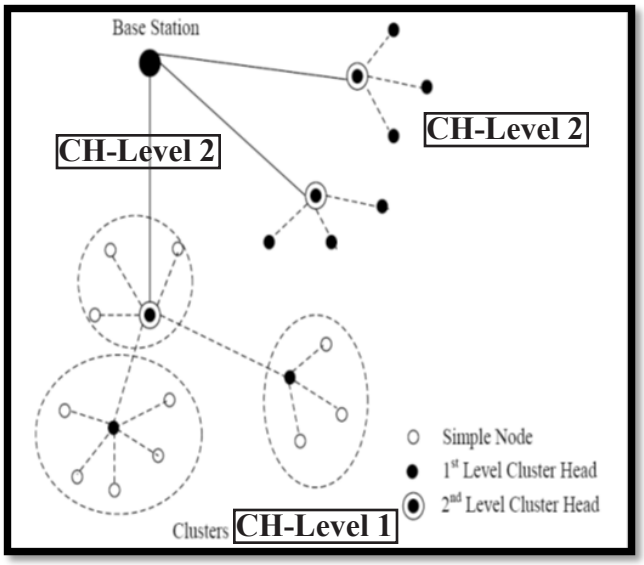

Figure: 1 Cluster Based Hierarchical Model

As shown in figure1 a hierarchical approach breaks the network into cluster layers. Nodes have been grouped into clusters with a cluster head which has the responsibility of routing from cluster to other cluster heads. Data generally travel from lower clustered layer to the higher one. Although it moves from one node to another, but which it moves from one layer to the other and it covers generally larger distances [11]. By this way it moves data faster. Clustering provides the inherent optimization capabilities at cluster heads. In this section, we review a sample of hierarchical-based routing produces for wireless sensor networks.

Low-Energy Adaptive Clustering Hierarchy (LEACH)

LEACH is a first and most popular energy-efficient clustering algorithm proposed for reducing power consumption in wireless sensor networks. The idea used in it is to form clusters of the sensor nodes based on the received signal strength and use local cluster heads as routers to the sink. By doing this we will save energy since transmissions has been done by cluster heads rather than all sensor nodes.

LEACH is based on the aggregation technique that combines on aggregation the original data into a smaller size of data that carry only meaningful information.

The operation of LEACH is been divided into two phases namely i.) A setup phase to organize the network into clusters, CH advertisement and transmission schedule creation and ii.) A steady state-phase for data aggregation, compression and transmission to sink.

LEACH is complete knowledge of network that reduces energy consumption by (a) minimizing the communication cost between sensors and their clusters heads and (b) turning off non-head nodes as much as possible [9].

And also LEACH terminates in a finite number of iterations; but does not guarantee for good CH distribution and also assumes uniform energy consumption for CHs.

Power-Efficient Gathering in Sensor Information System (PEGASIS)

PEGASIS is an extension of LEACH protocol, which forms a chain from sensor nodes so that each node transmits and receives from a neighbor's and only one node has been selected from that chain to transmit to the base station [10]. Gathered data moves from node to node aggregated and eventually sent to the base station .The chain construction is performed in a greedy way. As shown in Figure 2 node c0 passes its data to node c1. Node c1 aggregates node c0's data with its own and then transmits to the leader. After node c2 passes the token to node c4, node c4 transmits its data to node c3. Node c3 aggregates node c4's data with its own and then transmits to the leader. Node c2 waits to receive data from both neighbor's and then aggregates its data with its neighbor's data. Finally, node c2 transmits one message to the base station.

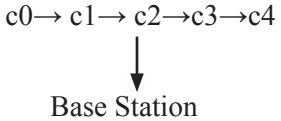

Figure: 2 Chaining in PEGASIS

Such a topology adjustment can introduce significant overhead especially for highly utilized network.

Hybrid-Energy Efficient Distributed Clustering (HEED)

HEED extends the basic scheme of LEACH by using residual energy for cluster selection to achieve power balancing [11]. HEED has been proposed with *four primary goals* namely (i) prolonging network lifetime by distributing energy consumption, (ii) terminating the clustering process within a constant number of iterations, (iii) minimizing control overhead, and (iv) producing well-distributed CHs and compact clusters.

In HEED the proposed algorithm periodically selects CHs according to a combination of two clustering parameters. The primary parameter is their residual energy of each sensor node (used in calculating probability of becoming a CH) and the secondary parameter is the intra-cluster communication cost as a function of cluster density or node degree (i.e. number of neighbors). The primary parameter is used to probabilistically select an initial set of CHs while the secondary parameter is used for breaking ties. However the cluster selection deals with only a subset of parameters, which are possibly constraint on system.

Threshold Sensitive Energy Efficient Sensor Network Protocol (TEEN)

TEEN is a hierarchical clustering protocol, which groups sensors with each led by a CH. The sensors within a cluster report to their CH.TEEN has been useful for applications where the users can control a trade-off between energy efficiency, data accuracy, and response time dynamically. However TEEN is not suitable for sensing application which is needed since the user may not get any data at all if the threshold is not reached.

Adaptive Periodic Threshold Sensitive Energy Efficient Sensor Network Protocol (APTEEN)

APTEEN is an improvement to TEEN and to overcome its shortcomings and aims at both capturing periodic data collections and reacting with time-critical events. The architecture of APTEEN is same as TEEN, which uses the concept hierarchical clustering for energy efficient communication between source sensors and sink.

It supports three different query types namely (i) historical query to analyze past data values, (ii) one-time query, to take a snapshot view of the network; and (iii) persistent queries, to monitor an event for a period of time.

VI. Location Based Protocols

In this location based protocol, sensor nodes are addressed by their locations. In this section, we present a sample of location-aware routing protocols proposed for wireless sensor networks.

Geographic and Energy-Aware Routing (GEAR)

GEAR is an energy-efficient routing protocol proposed for routing queries to target regions in a sensor field; GEAR uses energy aware heuristics that are based on geographical information to select sensors to route a packet to towards its destination region. Then GEAR uses a recursive geographic forwarding algorithm to disseminate the packet inside the target region.

Minimum Energy Communication Network (MECN)

MECN is a location- based protocol for a minimum energy for randomly deployed ad-hoc network, which attempts to set up and maintain a minimum energy network with mobile sensors.

In the first phase (encloses graph construction), MECN constructs a sparse graph, called an *enclosure graph,* based on the immediate locality of the sensors. An enclosure graph is a directed graph that includes all the sensors as its vertex set and whose edge set is the union of all edges between the sensors and the neighbors located in their enclosure regions. In other words, a sensor will not consider the sensors located in its relay regions as potential candidate forwarders of its sensed data to the sink. In the second phase (*cost distribution*), non-optimal links of the enclosure graph are simply eliminated and the resulting graph is a *minimum power topology.* This graph has a directed path from each sensor to the sink and consumes the least total power among all graphs having directed paths from each sensor to the sink.

To address this problem the enclosure graph and thus the minimum power topology should be dynamic based on the residual energy of the sensors.

Small Minimum-Energy Communication Network (SMECN)

SMECN is an routing protocol proposed to improve MECN, in which a minimal graph is characterized with regard to the minimum energy property. In SMECN protocol every sensor discovers its immediate neighbours by broadcasting a message with initial power that is updated incrementally. Specifically the immediate neighbors of a given sensor are computed analytically. Otherwise, it increments and rebroadcasts its neighbor's discovery message.

VII. Data Centric Protocols

Data centric protocols differ from traditional address-centric protocol in the manner that the data is sent from source sensors to the sink. In data-centric protocol when the source sensors send their data to the sink they can perform some form of aggregation on the data originating from multiple and send the aggregated data toward the sink.

Rumour Routing

Rumour routing is a logical compromise between query flooding and event flooding application schemes. Rumour routing is an efficient protocol if the number of queries is between two intersection points of the curve of rumor routing with those of query flooding and event flooding.

Rumour routing is based on the concept of agent, which is a long-lived packet that traverses a network and informs each sensor its network traverse. It also maintains and updates the event to maintain the shortest paths to the events that occur in the network.

COUGAR

The COUGAR routing protocol is a database approach to tasking sensor network. The COUGAR approach uses a query layer where every sensor is associated with a query proxy that lies between the network layer and application layer of the sensor. Since the COUGAR is a database approach it faces few challenges.

Active Query Forwarding in Sensor Network (ACQUIRE)

ACQUIRE is another data centric mechanism used for querying named data. It provides superior query optimization to answer very specific queries called one-shot complex queries for replicated data. ACQUIRE allows the queries to inject a complex query into the network and been forwarded through a sequence of sensors.

VIII. QOS Based Protocols

QOS protocols consider end-end delay requirements while setting up the paths in sensor network [12].

Sequential Assignment Routing (SAR)

It is the first protocol for sensor network that includes the notion of QOS in its routing decisions. This is also a multi-path approach [9]. The objective of SAR algorithm is to minimize the average weighted QoS metric throughout the lifetime of the network.

If topology changes due to node failures, a path re-computation is needed. As a preventive measure, a periodic re-computation of paths is triggered by the base-station to account for any changes in the topology.

SPEED

It is another QoS routing protocol for sensor networks that provides soft real-time end-to-end guarantees. SPEED does not consider any further energy metric in its routing protocol. Therefore, for more realistic understanding of SPEED's energy consumption, there is a need for comparing it to a routing protocol, which is energy-aware.

Energy-Aware QoS Routing Protocol

In this QoS aware protocol for sensor networks, real-time traffic is generated by imaging sensors. The proposed protocol extends the routing approach in and finds a least cost and energy efficient path that meets certain end-to-end delay during the connection. However, it does not provide flexible adjusting of bandwidth sharing for different links.

Conclusion

One of the main challenges in the design of routing protocols for WSNs is energy efficiency due to the scarce energy resources of sensors. In this paper, we have summarized recent research results on data routing in sensor networks and classified the approaches into three main categories, namely data-centric, hierarchical and location-based.

The factors affecting cluster formation and cluster-head communication are open issues for future research.

Moreover, the process of data aggregation and fusion among clusters is also an interesting problem to explore. We highlighted with the energy efficiency and the network challenges and its routing issues.

References

1. S.K. Singh, M.P. Singh, and D.K. Singh, "A survey of Energy-Efficient Hierarchical Cluster-based Routing in Wireless Sensor Networks", *International Journal of Advanced Networking and Application (IJANA)*, Sept.–Oct. 2010, vol. 02, issue 02, pp. 570–580.
2. S.K. Singh, M.P. Singh, and D.K. Singh "Energy-efficient Homogeneous Clustering Algorithm for Wireless Sensor Network", *International Journal of Wireless & Mobile Networks (IJWMN)*, Aug.2010, vol. 2, no. 3, pp. 49-61.
3. Jun Zheng and Abbas Jamalipour, "Wireless Sensor Networks: A Networking Perspective", a book published by A John & Sons, Inc, and IEEEE, 2009.
4. S. Misra et al. (eds.), *Guide to Wireless Sensor Networks*, Computer Communications and Networks,DOI: 10.1007/978-1-84882-218-4 4, Springer-Verlag London Limited 2009.
5. Ming Liu, Jiannong Cao, Guihai Chen, and Xiaomin Wang, "An Energy-Aware Routing Protocol in Wireless Sensor Networks", *Sensors* 2009, vol. *9*, pp. 445-462.
6. Luis Javier García Villalba, Ana Lucila Sandoval Orozco, Alicia Triviño Cabrera, and Cláudia Jacy Barenco Abbas, "Routing Protocol in Wireless Sensor Networks", *Sensors* 2009, vol. *9*, pp. 8399-8421.
7. E. Zanaj, M. Baldi, and F. Chiaraluce, "Efficiency of the Gossip Algorithm for Wireless Sensor Networks", In *Proceedings of the 15th International Conference on Software, Telecommunications and Computer Networks (SoftCOM)*, Split–Dubrovnik, Croatia, September, 2007.
8. Kemal Akkaya and Mohamed Younis, "A Survey on Routing Protocols for Wireless Sensor Networks", *Ad hoc Networks*, vol. 3, no. 3, May 2005, pp. 325-349.
9. W. Lou,"An Efficient N-to-1 Multipath Routing Protocol in Wireless Sensor Networks", *Proceedingsof IEEE MASS'05*,Washington DC, Nov. 2005,pp1-8.
10. X. Du and F. Lin, "Improving routing in sensor networks with heterogeneous sensor nodes",

Proceedings IEEE VTC'05, Dallas, TX, Sept. 2005, pp. 2528-2532.

11. Ossama Younis and Sonia Fahmy" Heed: A hybrid, Energy-efficient, Distributed Clustering Approach for Ad-hoc Networks", *IEEE Transactions on Mobile Computing*, vol. 3, no. 4, Oct.-Dec. 2004, pp. 366-369.
12. K. Akkaya and M. Younis, "An Energy-Aware QoS Routing Protocol for Wireless Sensor Networks,"in the Proceedings of the IEEE Workshop on Mobile and Wireless Networks (MWN 2003), Providence, Rhode Island, May 2003.

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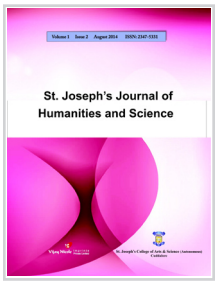

Mental Health of College Teachers

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Abstract

The present study aims to find out the mental health among the college teachers. 500 samples were selected randomly from engineering college teachers in and around Cuddalore district. Standardized psychological tool was used to collect the data. Statistical test t-test and One Way Anova (F-ratio) were used to test the hypotheses. Result was found that there is a significant difference in college teacher's mental health on the basis of gender and community.

Keywords: Mental health, self concept, self insight, self identity, self responsibility

Introduction

Health is a dynamic concept with multiple meanings that are dependent on the context in which the term is used. There is little doubt that people view health as essential to well being. However individual's definition of health vary according to their own social experience and are relative to their age, their personal knowledge, general knowledge, social and illness experience (Keleher and Macdoughal 2008).

Mental health is a balanced development of the individual personality and emotional attitudes which enable him to live harmoniously with his fellow men.

Health has been viewed in different perspectives by different culture over time. Despite the observation by the ancient Greek statements Pericles (495-429 BC) that "health is the state of moral, mental and physical well being which enable a person to face any crisis in life with the at most grace and facility".

The world health organization (WHO 1946) recognized "health as a state of complete physical, mental and social well-being and not merely the absence of disease or infirmity"

"Health is a state of complete physical, mental and social well-being and an ability to lead a socially and economically productive life" (OXFORD AND IBA NEW MEDICAL DICTIONARY 1990).

WHO declared that young people's mental health is a key area of concern to which professionals and policy-makers must direct their attention (WHO 2005). So, foundation for good mental health is laid in the early years of childhood and adolescence. Growing evidence

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shows the long-term value of promoting the positive mental health of children and young people.

Compared to adults, young people are especially at risk of creating vulnerabilities or developing mental health disorders as they face many new pressures and challenges in their daily lives. Leaving their parental home for the first time, financial worries, limited employment, new lifestyle development, educational opportunities or worries with human relations can cause high levels of stress, which can trigger mental disorder (WHO 2001).

Mental health of college students exhibit more severe mental illness. A study in (Science day August 13, 2010) severe mental illness is more common among college students. Young people are arriving on campus with pre-existing condition and willingness to seek help for emotional distress according to a study presented at 118th Annual convocation of (American Psychological Association 2010).

"Emerging evidence point out the increase in the prevalence of mental health problems among adolescents and later adolescents" (Surgeon General 1999).

Nature of Mental Health

The word mental pertains to the mind. It is a word which is seen almost exclusively in negative terms – as a term of abuse in the playground, at work and even in the family. But we are mental beings in the same; we are all 'physical beings. Mental health is as important as physical health if we are to grow and to flourish, if we are to contribute individually and collectively to the society, we need to accept that we are mental beings with emotional and spiritual needs, as well as physical ones to know the concepts of mental health following definitions given by expert may allow us to explore in this field.

Mental Health stated that of complete physical, mental and social well being, and not merely the absence of disease; also mental health is described to be an important one as physical health and playing a critical role for an individual's over all well- being. Today mental health problems are considered as one of the major public health concerns. The reported life time prevalence for any mental disorder varies between 33 % and 46%, (WHO 2006).

Definitions of Mental Health

According to Bernard (1970) mental health is in continuous adjusting rather than a static condition and is therefore a persuasive goal; it is an ability to cope with the present and in all likelihood to adjust satisfactorily in the future. It involves physical, mental and emotional phases of adjusting behavior as well as habits of work and attitude toward situation and obstacles.

According to Maslow (1948) mental health is "a condition, which permits the optimal development-physical, intellectual and emotional if the other individual, so far this is compatible with that of the individuals".

Hadifield (1950) defines "mental health as the full and harmonious functioning of the whole personality".

According to Kilander (1962) "Mental health is the measure of a person's ability to shape his environment to adjustment to adjust to life and he has to face it and to do so reasonable amount of satisfaction, success, efficiency and happiness."

Hence, mental health is a part of view one takes of all phases of living. The concept includes a social phase-socially considerate behavior, satisfaction with social order and contribution to society. Mental health is not simply the absence of disease but is a process of optimum functioning and maximum self realization.

Studies Related to the Topic

Nagai et al. (2007) studied poor mental health associated with job dissatisfaction among school teachers in Japan. Study aimed to compare the likelihood of having minor psychiatric disorders (MPD) among school teachers with that among civil servants, and to investigate what factors were specifically associated with MPD in teachers. Questionnaire – based survey of 403 teachers employed at state schools and 611 civil servants as a comparison group in a medium – sized city in Japan. In the group of civil servants, longer working hours, and physical illness were associated with an increased likelihood of having MPD. When this analysis was conducted separately for male and female teachers, job dissatisfaction alone was associated with teachers; job dissatisfaction alone was associated with MPD only in female teachers. Poor mental health of Japanese school teachers, female teachers in particular, was found to be associated with job dissatisfaction.

Khan and Beena [2008] explored the impact of mental health on the level of burnout of the teachers teaching at different education levels. Sample comprised 640 school and college teachers of four district of the eastern Uttar Pradesh. Burnout scale by Hatwal and Mithila and mental health status inventory by Anand Kumar and giridher were used; the obtained t-values 15.04,27.11 and 7.38 were found statistically significant at 0.01 level of confidence.

Dewan et al. (2009) examined the effects of gender, religion and marital status upon mental health of tribal school teachers in Jharkhand. A stratified random sample of 400 tribal school teachers was selected for the study. Results revealed that gender produces significant effects on mental health. Female teachers as compared to male teachers were found to show poor mental health. The main effects of religion on mental health were found to be significant. Christian school teachers as compared to saran teachers had better mental health. The effects of religion were same for male and female teachers and also for married and un-married teachers. Like-wise, the effects of gender were not different for married and un-married teachers.

Naik and Francis (2010) studied creativity in relation to mental health. The Population of study was all the class IX students reading in different schools of Sundargarh district. The sampling size of 150 students' comprising of 75 boys and 75 girls were selected for the study. Result of the study revealed that there was no significant relationship (r = -0.18) found between high creativity of students with their mental health. No significant relationship was found between low creativity of students with their mental health.

Balaji and Avaradi, [2013] conducted the following study on 100 adolescent studying in government and private colleges selected from couple of districts [gulgarga and yadagiri]; adjustment problems inventory and mental health inventory were administered on them; statistical t-test and correlation were employed for data analysis. It was found that there is a positive and significant correlation between adjustment problems and mental health of adolescents.

Methodology

Objectives

To analyse the significant difference among the engineering college teachers in their mental health on the basis of the demographic variables such as gender and community.

Hypotheses

- Respondents do not differ in their level of Mental Health on the basis of Gender.
- Respondents do not differ in their level of mental health on the basis of community.

Sampling and Sampling Method

500 samples from engineering college teachers in and around the Cuddalore District were selected by using random sampling techniques.

Method of Data Collection

The mental health inventory used in the research was developed by Augustine (7) consists of (60) items relating to various aspect of mental health namely self, other environment and life dimensions of self include acceptance of self insight, self identity, self responsibility, confidence and trust in oneself.

The second dimension is related to acceptance of warm and genuine relationship with others, feeling of emotional & Security, affection and love. The third dimension pertains to the perception of reality, personal freedom, healthy non-conformity open to experience and autonomous functioning. The fourth dimension is related to life which includes spontaneous free and natural living. Refined values, creativity and revelation of one's potential and life satisfaction. The questionnaire contains 15 items pertaining to each one of this dimension.

Statistical Tool Used

- Descriptive analysis
- Differential analysis
- The means, standard deviations of the entire sample are computed, In order to test the significance't' test is used. In order to find out the significance of more than two variables, 'F' test is also used in this present investigation.

Result and Discussion

Showing Mean , S.D, t-value for respondents level of Mental Health on the basis of Gender

	Gender	N	Mean	S.D	t-value	P-value
Mental Health	Male	243	83.99	6.39	4.86	0.001(S)
	Female	257	86.96	7.12		
	Total	500				

Source: Primary data

* Significant at 0.05 level

The above table exhibits the details of Mean, S.D. and t-value for respondents level of Mental Health on the basis of Gender.

It is inferred from the obtained t-value that there is a significant difference in respondents level of Mental Health on the basis of Gender. Since the calculated t-value (4.86) which is significant at 0.001 level. Therefore the stated null hypothesis is rejected and alternate hypothesis is accepted. Therefore it is concluded that respondents differ in their level of Mental Health on the basis of Gender. Hence female have higher mental health than male respondents. The present finding is supported by the previous study conducted by Dewan **et al. (2009).**

Showing Mean, S.D. and F-value for respondents level of mental health on the basis of community

	Community	N	Mean	S.D	F-value	P-value
Mental health	BC	26	93.54	24.12	10.1	0.001(S)
	MBC	276	84.74	7.66		
	SC	188	86.81	5.93		
	Others	10	91.00	0		
	Total	500	86.10	8.90		

Source: Primary data

* Significant at 0.05 level

The above table exhibits the details of Mean, S.D. and F-value for respondents level of mental health on the basis of community.

It is inferred from the obtained F-value that there is a significant difference in respondents level of mental health on the basis of community, since the calculated F-value (10.1) which is significant at 0.001 level. Therefore the stated null hypothesis is rejected and alternate hypothesis is accepted. Therefore it is concluded that respondents differ in their level of mental health on the basis of community.

Findings

- Respondents differ in their level of Mental Health on the basis of Gender. Female have higher mental health than male respondents.
- Result found that respondents differ in their level of mental health on the basis of community.

Recommendations

The following recommendations are suggested to improve the mental health of the college teachers.

1. Psychological counseling is to be arranged to know their strength and weakness and to cope with the stress and to maintain good mental health.
2. Stress management training is to be arranged to manage the stress.
3. Attitude change training program is to be given to create positive attitude.
4. Time management training is to be given to manage the time. Through these training programs every teacher can manage their time and plan effectively to perform their job successfully.
5. Positive thinking training will be given in order to improve mental health.

Conclusion

The present study aims to find out the significant difference in mental health among the engineering college teachers based on gender and community. 500 samples were selected randomly. Standardized Psychological tool was used to collect the data. Analysis reveals that Female have higher mental health than male respondents on the basis of gender. Further result also concluded that respondents differ in their level of mental health on the basis of community also.

References

Maslow (1948) A Report on Mental Illness Stigma, *American Health Association, USA.*

Hadifield, (1950). *Mental Health Promotion Working group of the Provincial Wellness Advisory Council* Canada: Mental Health Association,2007 by Heather Pollett.

Kilander, (1962). *Mental Health Promotion Working group* of the Provincial Wellness Advisory Council, Mental Health Association,2007 by Heather Pollett, Canada.

Bernard, W. H.W. (1970). *Mental Health of Children in Class Room New York:* Mc Graw Hill Publication.

Nagai et al. (2007) Teacher burnout in relation to mental health. Edutracks, 7(9): 31-33.

Dewan (2009) Mental Health and Academic Success in College revised and resubmitted to the *B.E. Journal of Economic Analysis & Policy.*

Naik and Francis (2010) *Mental Health and Work: Issues and Perspectives*. Adelaide, Auseinet: The Australian Network for Promotion, Prevention and Early Intervention for Mental Health.

Balaji, & Avaradi, (2013). Study on Adjustment Problem and Mental Health, *International Conference Reports,* Drawad: Karnataka University.

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Page 1

Title of paper: max 20 words (make it short, yet descriptive); avoid abbreviations

Name of Author, Designation and Official Address. (if more than 1 author use superscript [1],[2])

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"**Abstract**" Body of abstract (summary of contributions and/or results; approx. 1 line per page)

"*Keywords:*" followed by 5 to 10 keywords and key phrases describing the content

Pages 2 – *k*

"**1. Introduction**"

Give background on the topic (provide context and include references on prior work), justify your interest in the topic, prepare the readers for what they will find in later sections, and summarize (in a few sentences) your main findings and/or contributions. This section must be kept short. If it exceeds, say, 3 pages, you may wish to break it up by including an additional section that covers the *necessary* details for one or more of the above aspects. Use a descriptive title such as "**2. Review of Prior Work**" or "**2. Notable Applications of** ... " for this section.

Pages (*k*+1) – *l*

Body of the paper should consist of sections dealing with various aspects of the investigation as appropriate; e.g., theory, applications, design issues, tradeoffs, evaluation, experiments, comparisons with other methods or approaches. Don't be afraid to compare, criticize, and generally leave your personal mark on the paper. There is no general rule, except that subdivisions must be coherent and of reasonable length. Avoid the extremes of single-paragraph and 5-page sections. For very long sections, consider dividing up or moving some details to an appendix.

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Give a brief summary (in a few sentences) of what has been presented and/or accomplished. Emphasize the advantages and disadvantages of the proposed approach, technique, or design. Discuss possible extensions of the work and any interesting/open problem that you can envisage. Like the **Introduction**, this section must be fairly short.

Pages (m+1) – n **"References"**

Provide complete bibliographic information for each reference (see any paper in *IEEE Trans. Computers* for examples). As a rule of thumb, citing 5-20 references is reasonable; review or survey-type papers tend to have much more extensive bibliographies and original contributions breaking new ground may have fewer references.

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