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By G. S. Anagnostatos

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Keywords: neutron nuclei, ^4n-^{16}n, Isomorphic Shell Model.

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SEARCHINGFORPOSSIBLESTABILITYIN1S1PAND1D2SNEUTRONSHELLS

Strictly as per the compliance and regulations of :

Searching for Possible Stability in 1s, 1p, and 1d2s Neutron Shells

G. S. Anagnostatos

Abstract- The Isomorphic Shell Model is applied to the first three neutron shells in searching for possible stability there It has been found that the even neutron nuclei ^{4}n – ^{16}n show possible stability, some of which exhibit stable excited states as well.

Keywords: *neutron nuclei,* ^{4}n-^{16}n, *Isomorphic Shell Model.*

I. Introduction

The production and detection of free neutron clusters (an entirely new form of nuclear matter) have been seriously studied, initially through the channel Be= Be+ n [1].Other supporting n experiments involve the reactions ^{12}Be=^{8}Be+^{4}n [2] and ^{8}He=^{4}He +^{4}n [3]. In [4] a review is made and the far-reaching implications of ^{4}n are discussed.

Neutron nuclei heavier than ^{4}n have been studied, specifically ^{8}n in the decay of ^{252}Cf [5] and $^{5-13}$n in induced fission of ^{235}U [6]. All these efforts lasting for decades have set the question: Can a nucleus be made up of neutrons alone?

From the theoretical point of view [7-8], it does not seem possible to bind ^{4}n without destroying many other successful predictions by applying the same forces, e.g., to light nuclei. However, simulations in progress are used to clarify the origin of ^{4}n by employing the Generator Coordinates Method and locating the neutrons at the vertices of a tetrahedron .

A recent publication [9] favours the possible stability of ^{4}n and ^{6}n in the framework of the Isomorphic Shell Model (ISM). In the present work we employ the same model to study the possibility of stability of neutron nuclei in the next 1d2s shell. In order to correct a small numerical mistake in the results of [9], the present research repeats the study of 1s and 1p neutron nuclei. The privilege of the present approach is that while the model has been successfully applied throughout the periodic table [10-19], here the model is employed without any modification, constituting the model unique In the relevant research.

II. The Isomorphic Shell Model (ISM)

The model follows the sequence of reasoning based on well documented quantum mechanical

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principles and mathematical theorems

- The nucleus is composed of two different kinds of fermions (neutrons and protons).
- The wave function describing neutrons or protons or both is anti-symmetric.
- Anti-symmetric wave function of a set of particles (e.g.,nucleons or protons) has maximaat positions which are identical to those positions if the particles interact among eachother via a repulsive force of unknown nature[20].
- Repulsive particles on a sphere are at equilibrium only for specific numbers of particleswhich are identical to the number of vertices, or to the number of faces, or to the numbersof middles of edges or combinations of these numbers related to the regular or semi-regular polyhedra [21].
- Two kinds of repulsive particles (here, neutrons and protons) are at equilibrium on asphere if the neutrons by themselves are at equilibrium and if the protons by themselvesare at equilibrium, and if all these particles taken together are at equilibrium aswell [21].
- If the number of repulsive particles is larger than the aforementioned numbers [21], thenThe extra particles could be at equilibrium on a different sphere which does not disturb theequilibria of particles on other spheres [21].2

The first three of the aforementioned cornerstones of the model come directly from basic quantum mechanics and the other three are rigorously proved mathematical theorems [21]. *No ad hoc assumption is introduced anyhere.* This is the outstanding, unique privilege of the present model.

By rigorous application of the above principles and theorems, the most probable forms of nuclear shells are derived for the whole periodic table of nuclei, i.e., up to Z=126 and N=184 [22]. If in addition the nucleons are considered with finite size (specifically, r_p = 0.860 fm and r_n = 0.974 fm), then the average size of all shells are derived by considering packing of the shells assumed superimposed with a common center and the most symmetric relative orientation [22] (packing means that the bags of a polyhedron come in contact with the bags of a previous polyhedron). Thus, in the ISM the most probable forms and the average sizes of the nuclear shells, and thus of all nuclei, are determined without reference to nuclear forces.

Thorough study of regular and quasi-regular polyhedra employed by the present model shows that the symmetries of these polyhedra identically possess the quantization of orbital angular momentum, of spin, and of total angular momentum [23], a fact which permits one to assign quantum states at the vertices of these polyhedra assumed as the average particle positions. Each occupied vertex configuration corresponds to a quantum state configuration with definite quantum state and energy.

In general, the ISM is a microscopic nuclear structure model that incorporates into a hybrid model the prominent features of single-particle and collective approaches in conjunction with the nucleon finite size [24]. The model consists of two parts, namely, the complete quantum mechanical part [24] and the semiclassical part [24, 25].

Figure 1 stands for the shell structure for all nuclei up to N = Z =20 according to the ISM [12-14]. Thus, the first three neutron and the first three proton shells are shown. This is a good way to see the relationship between regular nuclei and possible neutron nuclei. Polyhedral vertices, standing for nucleon average positions in definite quantum states (τ, n, ℓ, m_ℓ, s), are numbered as shown. Central axes standing for the quantization of directions of the orbital angular momentum are labelled as and pass through the points marked by small solid circles •. At the bottom-left of each block the numbering of a polyhedron proceeded by the letter Z (N) for protons (neutrons) is given. Over this the number of polyhedral vertices and the number of possible unoccupied vertices (holes, h) are also given. At the bottom-right of each block the radius of the polyhedron is listed. Over this the cumulative number of vertices of all previous polyhedra and of this polyhedron is also given and stands as a quantum-geometrical interpretation of magic numbers. Finally, at the bottom-center of each block the distance $P_{n\ell m}$ of the nucleon average position nℓm from the relevant axis is given. The coordinates of nucleon average positions of Fig.1 have been determined [11] and are identically employed in all publications thereafter {e.g., [12-14].

At this point it is interesting for one to observe from Fig. 1 that the average structures of a neutron and of the corresponding proton shell on the same line of this figure are presented by reciprocal polyhedra [26]. That is, the average positions of protons (neutrons) are at the directions through the centers of the faces of the corresponding neutron (proton) polyhedron, thus these two polyhedra possess the same rotational symmetry. This relative orientation makes the np distances systematically smaller than the nn and the pp distances. This situation,2even using the same r- dependent potential as in Eq.(1) below, leads to a much stronger total average np interaction.

Apparently, if we are concerned with neutron nuclei alone, consideration of only the neutron polyhedra of Fig.1 is enough. It is important to emphasize that the neutron polyhedrapossess *stable* equilibrium for repulsive particles possessing average positions at their vertices, while proton polyhedra possess *unstable* equilibrium [21]. Thus, neutron polyhedracan exist by themselves, as far as their stability is concerned. Even their average sizes areindependent from the existence of proton polyhedra. Specifically, the octahedron standing forthe 1p neutron shell is closely packed with the neutron zerohedron standing for the 1s neutronshell. Similarly, the icosahedron standing for the 1d2s neutronshell is closely packed with the aforementioned octahedron.

III. SEMI-CLASSICAL VERSION OF THE ISM

Here, we present the semiclassical part of the model,which has been used many times [12-14] in place of the quantum mechanical part of themodel [24], in the spirit of the Ehrenfest theorem [27, 28] that for the average values the laws of Classical Mechanics are valid [28].

In the present semiclassical treatment, we employ Eqs. (1-5) as the expression of thetwo-body (two Yukawa) potential V [16, 29], of the kinetic energy T [11], of the spin-orbitenergy V_{LS} [30], and of the binding energy (E_B). Isospin term in Eq.(5) is not needed since the isospin is here taken care of by the different shell structure (forms and sizes) betweenproton and neutron shells, as apparent from Fig.1.

$$V_{ij}=1.7*10^{17}*e^{-31.8538r_{ij}}/r_{ij}-241.193*e^{-1.4546r_{ij}}/r_{ij} \quad (1)$$

$$<T>_{n\ell m}=(\hbar^2/2M)[1/R^2_{max}+\ell(\ell+1)/\rho^2_{n\ell m}] \quad (2)$$

$$\Sigma_i V_{LiSi}=\lambda \Sigma_i *(\hbar\omega_i)^2/(h^2/m)*\ell_i s_i \quad (3)$$

$$\hbar\omega_i = (\hbar^2/M)(n+3/2)/<r_i^2> \quad (4)$$

$$E_B.= \Sigma_{ij}V_{ij} - \Sigma<T>_{n\ell m} - \Sigma_i V_{LiSi} \text{ , where:} \quad (5)$$

- V_{ij} is the potential energy between a pair of nucleons i, j at a distance r_{ij}.
- $<T>_{n\ell m}$ is the average kinetic energy of a nucleon at the quantum state n, ℓ, m and consist of two terms. The first is due to uncertainly and the second to orbital motion of this nucleon.
- n, ℓ, m are the quantum numbers characterizing a polyhedral vertex standing for the averageposition of a nucleon at the quantum state n, ℓ, m.
- ℓ_i and S_i stand for the orbital angular momentum quantum number ℓ and the intrinsic spinquantum number s of any nucleon i.
- M is the mass of a proton M_p or of a neutron M_n,
- R_{max} is the outermost proton or neutron polyhedral radius (R) of a nucleus plus the relevantaverage nucleon radius r_p for a proton and r_n for a neutron (i.e., Rmax is the radius of thenuclear volume in which protons or neutrons are confined),

- $P_{n\ell m}$ is the distance of a nucleon average position at a quantum state (n, ℓ, m) from its orbital angular momentum vector at the direction $_n\theta^m_\ell$.

When only binding energies (and not scattering properties) are required as here, just the second term of the above two-body potential of Eq.(1) is sufficient. Thus, for non-scattering

properties, the parameters of the model are the following five: the two-size parameters R_p and R_n, the two parameters from the second term of Eq.(1), and the one parameter, λ, from Eq.(3). With the help of these *universal* (i.e., they are not adjustable and thus they maintain the same values for all properties in all nuclei) parameters all quantities R_{max}, $P_{n\ell m}$, and $\hbar\omega_i$, in Eqs.(1) – (5) are obtainable by employing the coordinates of the nucleon average positions derived from Fig.1 [12-14] and are given in [11].

IV. Application to Neutron Nuclei

If only neutrons are considered, the relevant shell structure is derived from Fig.1 by disregarding the proton shell structure.

Application of Eqs. (1-5) for neutron nuclei leads to the results shown in Table 1. Specifically, in its columns 1-9 we give the notation of a nucleus with even number of neutrons, the average positions of Fig. 1 occupied, the relevant state configuration, the quantities ΣV_{ij}, $\Sigma<T>_{n\ell m}$, ΣV_{LiSi}, E_B, the notations stable or unstable, and the average radius of each nucleus, respectively. From column 8 of Table 1 we see that the nuclei ^{4}n- ^{16}n have at least one state with positive E_B, a fact which implies that they are possible stable neutron nuclei. It is noticeable that several of these nuclei, besides their ground state, show stability for one or more excited states. It is of interest that when ^{8}n is a closed shell nucleus its E_B is negative, while if we consider 2p-2h (i.e., their core is ^{12}C and not ^{16}O) the ^{8}n has positive E_B. This, of course, is consistent with the structure of ^{16}O where for its ground state we have 4p-4h structure [24]. From preliminary calculations the same situation occurs for ^{18}n and ^{20}n. That is, while for these two nuclei their E_B in Table 1 have a negative sign, after considering p-h structure with the next shell their E_B becomes positive. That is, this situation implies that neutron nuclei could be possible even for the next 1f2p shell. Another interesting comment from the results of Table 1 is that the configurations possessing 2s states have larger positive E_B than the other configurations of the same nucleus without 2s states.

Figure 2 shows the space arrangement of neutrons for all neutron nuclei examined and listed in column 1 of Table 1 following the average positions Nos from column 2 of the table.

Table 2 shows the same quantities like Table 1 for the regular nuclei ^{4}He and ^{40}Ca, i.e., the nuclei with N = Z corresponding to the first and the last possible

neutron nuclei of Table 1 by employing identically as above the same equations and parameters. In addition this table deals with charge and point neutron – point proton rms radii. Here, the existence of experimental values for binding energies and radii and their impressive closeness to the present predictions give necessary credits to the model employed and to predicted possible neutron nuclei.

The necessary formulae for the radii are

$$<r^2>_p = \frac{\Sigma_1^Z r_i^2}{Z} + <r^2>_p - 0.116\frac{N}{Z} \text{ and} \qquad (6)$$

$$<r^2>_n = \frac{\Sigma_1^N r_i^2}{N} + <r^2>_n, \qquad (7)$$

Where the first is for the calculation of proton rms radii and the second for the estimation of neutron radii. The radii r_i are the radii R_i from Fig.1. The quantity $<r^2>p$ is taken as 0.8^2 fm^2 and presents the square of the average size of a proton, while the proton bag radius is already given above equal to 0.860 fm. In correspondence for the neutron we take 0.91 fm as the average size of a neutron, while the neutron bag radius, as given above, is 0.974 fm. The 5 quantities 0.8fm and 0.91fm have some minimum contribution to the radii only to the results of protons or neutrons rms radii of very light nuclei.

The values of neutron radii given in column 9 of Table 1 come as results of applying Eq.(7) above.to the average positions of neutrons given in column 2 for all nuclei of column 2 of Table 1.

V. Conclusions

From the ten even neutron nuclei examined in Table 1, seven show the possibility of having at least one state with positive E_B. From the remaining three nuclei of this table the ^{2}n definitely has negative E_B, while the other two, namely ^{18}n and ^{20}n, from preliminary calculations are expected to obtain positive E_B through a p-h structure with the next 1f2p shell. From the nuclei with positive E_B, namely, ^{4}n-^{16}n, the ^{4}n, ^{6}n, and ^{16}n have only one state with positive E_B. The nuclei ^{8}n, ^{12}n, and ^{14}n have two states with positive E_B, while the nucleus ^{10}n has four states with positive E_B.

It is noticeable that ^{8}n and ^{20}n, even though closed shell nuclei, do not exhibit positive E_B. This is here understood as a result of the structure of ^{2}n (i.e., the neutron zerohedron) which favours prolate structures. Thus, the states 1p1/2 and 1d3/2 with average positions towards the z axis, which is perpendicular to the neutron zerohedron, are less favoured. The same explanation is valid for ^{18}n which also possesses 1d3/2 states in its structure.

It is important to emphasize that the present calculations have the following characteristics:
a) They employ the same model already successfully applied to many calculations of regular nuclei with very good results [10-16, 19, 22-25], a model based

b) While the two-body potential employed here [Eq.(1)] has been strictly derived from nuclear physics [16, 29], it is almost identical to potentials derived from particle physics via chromodynamics.

c) The radii in column 9 of the table for possible neutron nuclei are identical to the neutron radii of regular nuclei with neutrons at the same quantum states [23].

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Table 1 : Energy components and rms charge and point neutron - proton radii (in fm) of 4He and 40Ca

Nuc.	Pos.	Config.	ΣV	$\Sigma<T>$	E_c	E_R	$E_{B.m}$	$E_{B,e}$	$_{ch}<r^2>^{1/2}m$	$_{ch}<r^2>^{1/2}e$	$_n<r^2>^{1/2}-_p<r^2>^{1/2}$	
4Hε	1-4	$(1s)^4$	44.6	14.2	0.5	1.7	28.2	28.3	1.71	1.68		
40Ca	1-40	$(1s)^4(1p)^{12}$ $(1d)^{20}(2s)^4$	771.7	363.0	64.8	1.7	342.2	342.1	3.47	3.48	-0.29	-0.30

Table 2 : Calculations of binding energies (in MeV) and radii (in fm) for the nuclei listed in the first column of the table. 8

Nuc	Average positions Nos.	State configurations	ΣV	$\Sigma<T>$	ΣE_{s-}	E_B	st. un.	Rad.
^{2}n	1-2	$(1s1/2)^2$	7.27	10.93	0.00	-3.66	un.	1.33
^{4}n	1-2, 7-8	$(1s1/2)^2(1p3/2)^2$	23.13	-19.98	0.20	**3.35**	st.	2.11
^{6}n	1-2, 5-8	$(1s1/2)^2(1p3/2)^4$	40.53	-36.55	0.39	**4.37**	st.	2.31
^{8}n	1-2, 5-10	$(1s1/2)^2(1p3/2)^4(1p1/2)^2$	50.79	-53.12	0.00	-2.33	un.	2.41
	1-2, 5-8, 25, 27	$(1s1/2)^2(1p3/2)^4(1d5/2)^2$	61.02	-54.60	0.58	**7.00**	st.	2.72
		$(1s1/2)^2(1p3/2)^4(2s1/2)^2$	61.02	-48,13	0.39	**13.28**	st.	2.72
^{10}n	1-2, 5-10, 25, 27	$(1s1/2)^2(1p3/2)^4(1p1/2)^2(1d5/2)^2$	71.67	-69.77	0.19	**2.09**	st.	2.71
		$(1s1/2)^2(1p3/2)^4(1p1/2)^2(2s1/2)^2$	71.67	-63.30	0.00	**8.37**	st.	2.71
	1-2, 5-8, 25-28	$(1s1/2)^2(1p3/2)^4(1d5/2)^4$	79.22	-76.87	0.77	**3.12**	st.	2.94
		$(1s1/2)^2(1p3/2)^4(1d5/2)^2(2s1/2)^2$	79.22	-70.40	0.58	**9.40**	st.	2.94
^{12}n	1-2, 5-10, 18, 20, 25, 27	$(1s1/2)^2(1p3/2)^4(1p1/2)^2(1d5/2)^4$	90.96	-92.03	0.38	-0.69	un.	2-90
		$(1s1/2)^2(1p3/2)^4(1p1/2)^2(1d5/2)^2(2s1/2)^2$	90.96	-85.56	0.19	**5.59**	st.	2.90
	1-2, 5-8, 18, 20, 25-28	$(1s1/2)^2(1p3/2)^4(1d5/2)^6$	97.32	-99.13	0.72	-1.09	un.	3.08
		$(1s1/2)^2(1p3/2)^4(1d5/2)^4(2s1/2)^2$	97.32	-92.66	0.77	**5.43**	st.	3.08
^{14}n	1-2, 5-10, 17-20, 25, 27	$(1s1/2)^2(1p3/2)^4(1p1/2)^2(1d5/2)^6$	110,82	-114.29	0.56	-2.91	un.	3.02
		$(1s1/2)^2(1p3/2)^4(1p1/2)^2(1d5/2)^4(2s1/2)^2$	110.82	-107.82	0.38	**3.38**	st.	3.02
	1-2, 5-8, 17-20, 25-28	$(1s1/2)^2(1p3/2)^4(1d5/2)^6(2S1/2)^2$	115.99	-114,92	0.96	**2.03**	st.	3.17
^{16}n	1-2, 5-10, 17-20, 25-28	$(1s1/2)^2(1p3/2)^4(1p1/2)^2(1d5/2)^6(2s1/2)^2$	130.52	-130.09	0.56	**0.99**	st.	3.11
^{18}n	1-2,5-10,17-20, 21,23,25-28	$(1s1/2)^2(1p3/2)^4(1p1/2)^2(1d5/2)^6(2s1/2)^2(1d3/2)^2$	150.96	-152.35	0.28	-1.11	Un	3.18
^{20}n	1-2, 5-10, 17-28	$(1s1/2)^2(1p3/2)^4(1p1/2)^2(1d5/2)^6(2s1/2)^2(1d3/2)^4$	171.96	-174.61	0.00	-2.65	Un	3.23
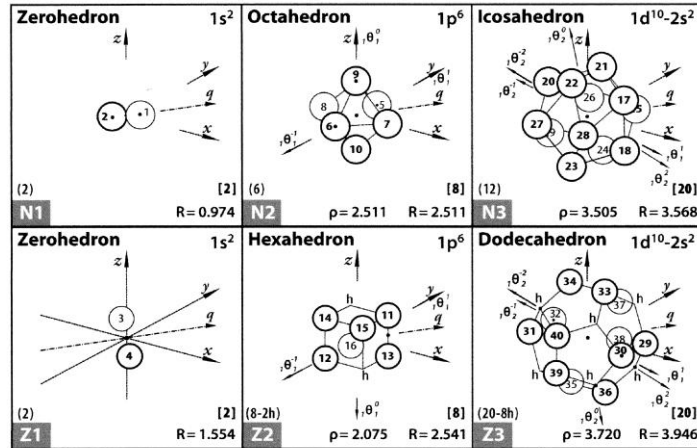
Fig.1

Figure 1 : Most probable forms and average sizes of the first three neutron and the first three proton shells up to N=Z=20
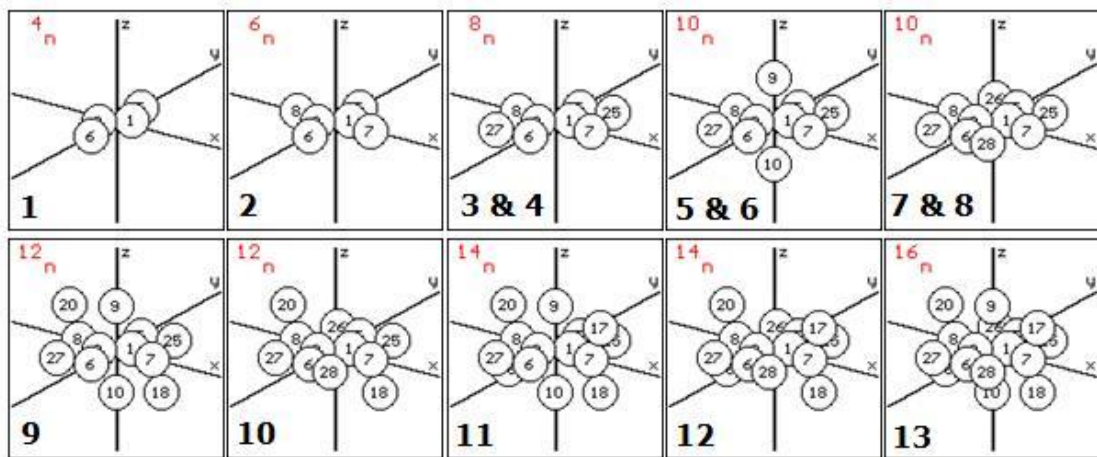
Figure 2 : Most probable forms and average sizes of possible neutron nuclei according to Table 1 following the numbering of column 4. From this column we can see that the same number may correspond to more than one state configurations shown in column 3 of the table. The numbering of bags in this figure corresponds to the numbering of bags in Fig. 1. That is, it specifies the same point in space.

Sorption of Ni^{2+} Ions by Anion Exchangers based on Epichlorohydrin Oligomers and 4-Vinylpyridine

By A. Pidakhmet, E. E. Ergozhin, T. K. Chalov & A. I. Nikitina

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Abstract- The new anion exchange resin (OECH-VP) was synthesized by polycondensation of oligomer epichlorohydrin (OECH) and 4-vinylpyridine (VP), the static exchange capacity (SEC) of which is equal to 6.75 mg-equiv g^{-1} in 0.1 M HCl solution and the sorption of Ni^{2+} ions were studied. The influence of the concentration and pH of the Nickel (II) sulfate *heptahydrate* solutions, contact time on the sorption activity of new anion exchangers (ECHO-VP) to nickel ions were studied. Structure of the surface anionite was studied by electronic microscopy method.

GJSFR-B Classification : FOR Code: 259999p

SORPTIONOFNIIIONSBYANIONEXCHANGERSBASEDONEPICHLOROHYDRINOLIGOMERSANDHVINYLPYRIDINE

Strictly as per the compliance and regulations of :

Sorption of Ni^{2+} Ions by Anion Exchangers based on Epichlorohydrin Oligomers and 4-Vinylpyridine

A. Pidakhmet [α], E. E. Ergozhin [σ], T. K. Chalov [ρ] & A. I. Nikitina [ω]

Abstract- The new anion exchange resin (OECH-VP) was synthesized by polycondensation of oligomer epichlorohydrin (OECH) and 4-vinylpyridine (VP), the static exchange capacity (SEC) of which is equal to 6.75 mg-equiv g^{-1} in 0.1 M HCl solution and the sorption of Ni^{2+} ions were studied. The influence of the concentration and pH of the Nickel (II) sulfate heptahydrate solutions, contact time on the sorption activity of new anion exchangers (ECHO-VP) to nickel ions were studied. Structure of the surface anionite was studied by electronic microscopy method.

I. Introduction

The problem of extracting Ni^{2+} ions is an actual when purifying wastewater of mining and metallurgical and engineering industries from them for example, when processing copper-nickel ore [1], sewage of nickel plating plants [2, 3] and others. Nickel is widely used in technology as anti-corrosion coatings, it is part of many non-ferrous alloys [4]. Production of nickel from oxidized nickel and sulfide ores is accompanied by formation of large amounts of waste water, which leads to water pollution [5]. Thus, the coefficient of accumulation of nickel by hydrobionts (the ratio of concentration of pollutants in the organism of a hydrobiont to its concentration in the aqueous medium) reaches 85-235.

In this regard, high requirements to methods of its removal from industrial wastewater are obvious. One of the promising methods for separation and concentration of microquantities of elements is the sorption extraction from solutions by polymer complex forming sorbents [6,7]. Therefore, an actual objective is to obtain ion exchangers based on the available materials and having high sorption properties with respect to nickel ions.

An important direction in practical application of ion exchange materials is purposeful synthesis of new selective sorbents and improvement of characteristics of known synthetic materials by introduction (into the sorbent matrix) of functional groups capable of reacting with metal ions to form complexes and chelates or ion associates.

In this study, we synthesized and characterized of anion exchangers OECH-VP-I and OECH-VP -II based on epichlorohydrin oligomer (ECHO) and 4 – vinylpyridine (VP).

II. Experimental

a) Reagents and materials

Epichlorohydrin (ECH) (99 %, empirical formula C$_3$H$_5$ClO, Mw 92.52 g mol^{-1}, density 1.183 g/ml at 25°C, boiling point 115-117°C, melting point -57°C, refractive index n 20/D 1.438 Sigma-Aldrich, Germany).

4-vinylpyridyne (VP) (95 %, Empirical formula C$_7$H$_7$N, Mw 105.14 g mol^{-1}, density 0.975 g/ml at 25°C, boiling point 62-65 °C, refractive index n 20/D 1.549 Sigma-Aldrich, Germany).

Benzoyl peroxide (BP) (Linear formula (C$_6$H$_6$CO)$_2$O$_2$, Mw 242.23g mol^{-1}).
Nickel (II) sulfate heptahydrateNiSO$_4$·7H$_2$O.

Epichlorohydrin oligomer (ECHO) was obtained in the presence of the M-14 catalyst, activated aluminosilicate (H$^+$ + Al^{3+}), taken in an amount of 1%of the monomer weight. The reaction mixture washeated for 2 h at 30 -50°C and for 5-6 h at 60-80°C with stirring at a constant rate and then cooled down. The reaction product was dissolved in benzene, precipitated with water-ethanol mixture (2:1), and filtered off. The resulting viscous brown product was dried at room temperature under vacuum to constant weight.

Anion exchange resin was synthesized in an optimalcondition by polycondensation of epichlorohydrin oligomer (ECHO) and 4-vinylyridine (VP) in the presence of 0.1-0.5 wt.% benzoyl peroxide at 80 °C for 5 hours in a weight ratio ECHO:VP equal to 10:4. Then the reaction mixture is cured at 120°C for 16 hours. It was then ground to give a particle size of 0.5-1.0 mm. As a result, a new anion exchanger ECHO-4VP was synthesized.Thespatialstructureoftheanionexchangerresin:

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$$OH-CH_2-CH-O-CH_2-CH-CH_2-\overset{+}{CH}-O-CH_2-\overset{\overset{\displaystyle Cl}{|}}{\underset{\displaystyle CH_2}{CH}}-O-CH\text{-----}R^-$$

(chemical structure diagram)

b) Study of thesorption of nickel (II) ions by anion exchangers

For preparation of model solutions the salt NiSO₄·7H₂O of analytical grade was used qualification. The concentration of nickel sulphate solutions varied from 0.165 to 2.099 g/L and the acid - in the range of pH from 1.5 to 6.9 with addition of 0.1N H₂SO₄ solution or NaOH. The contact of sorbents with NiSO₄ solution ranged from 1h up to 7 days. Sorption capacity (SC) was calculated from the difference between the initial and equilibrium concentration of the solutions, which were determined by classical polarography on the background of 0.5 M NH₄Cl on waves recovery Ni²⁺ (E₁/₂ = −1.07V).

III. Results and Discussion

The effect of concentration and pH of model solutions of NiSO₄ and their contact time on sorption of Ni²⁺ ions by new anion exchangers based on epichlorohydrin oligomer and 4-vinylpyridine (Fig.1-3) was studied.

Figure 1 : Isotherms of Ni²⁺ ions sorption by anion exchangers OECH -VP-I (1) and OECH -VP-II (2), the contact time is 7 days

Figure 2 : Dependence of sorption of Cu^{2+} ions by anion exchanger OECH -VP-I on acidity of $NiSO_4$ solutions (C_{Ni}= 2g/L, contact time is 7 days)

As is seen in Figure.1, anion exchanger OECH-VP-I absorbs Ni^{2+} ions much better than OECH-VI-II, which is consistent with their values of SEC. When extracting them from $NiSO_4$ solution containing 2.1 g / l of nickel, the SC is for them respectively 346.4 and 276.0 mg / g.

One of the important factors influencing the sorption characteristics of ion exchangers is acidity of

solutions. The maximum absorption of Ni^{2+} ions by anion exchanger OECH-VP-I was observed at pH 5.2 (Fig. 2). As follows from Fig. 3, it takes 6 hours to reach the equilibrium state between the anion exchanger OECH-VP-I and a solution of $NiSO_4$, containing 2.1 g/L of nickel and having pH 5.2.
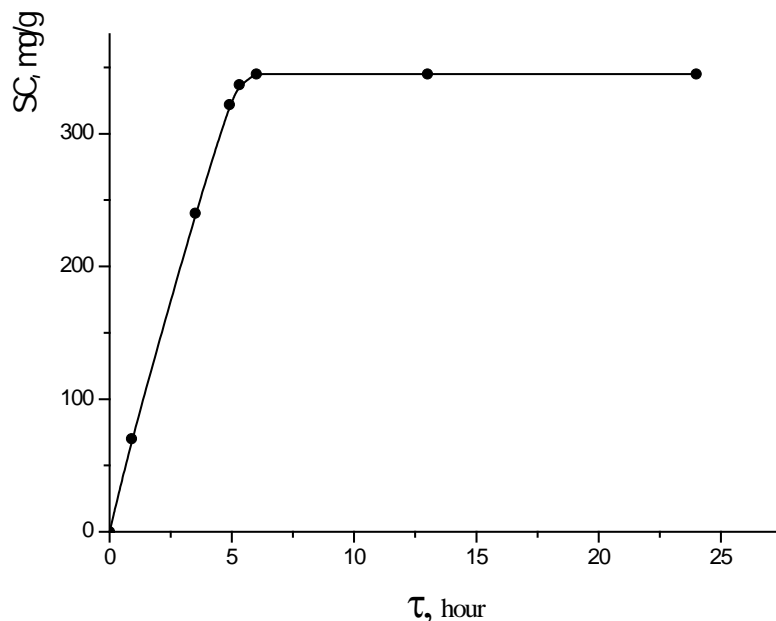
Figure 3 : Kinetic curves of sorption of Ni^{2+} ions by anion exchanger OECH-VP-I (1) from $NiSO_4$ solution (C_{Ni}=2,1g/L, pH 5.2)

The authors [8] in the study of the sorption of Ni^{2+} ions from solutions, containing 100 mg/L (pH 5.5), by industrial weak basic anion exchangers AV-17, AN-

31, AM-7 and AN-221 stated that their SC is respectively 0.021, 0.162, 0.219 and 0.278 mg-eq/g.

When extracting Ni^{2+} ions from 0.005 N solution of the mixture of copper, nickel and cobalt sulfates by anion exchangers based on allyl bromide, OECH and polyethyleneimine or polyethylenepolyamine, SC by Ni^{2+} ions reaches 0.67 mg-eq/g [1]. The exchange capacity of the polyelectrolyte based on glycidyl methacrylate and poly-2-methyl-5-vinylpyridine by nickel does not exceed 45 mg/g or 1.53 mg-eq/g [9].

Sorption characteristics of anion exchangers are known [6,7] to depend on the concentration of solutions. It was found that, when extracting Ni^{2+} ions from $NiSO_4$, solutions containing 0.16; 0.50 and 2.10 g/L, SC of anion exchanger OECH-VP-I is respectively 2.32; 4.61 and 11.80 mg-eq/g. Comparison of the results with the literature data shows that the SC of synthesized anion exchanger based on OEHG and 4-vinylpyridine is much higher than that of the known and industrial anion exchangers.

It is known [10] that the topological structuregiven bythe chemical structure of the initial monomersandthe synthesis conditionsplays an importantrole inshaping the properties ofcross-linked polymer.The affinityto theanion exchange resinsof complexingmetal ionsdepends on theirporosity andelectron donatingcapabilityof the functionalgroups [11]. Fig.4shows thesurface morphology ofthe anion-exchangerOECH-VI-I. These electrons microscopic analysisshowedthe anion exchangeratOECH-VI-I it is presentedin the formof straightfolds.

The anion exchangerhasa developed systemof macropores. As seen fromFig. 4their sizesOECH-VI-I are within0.698-1.764microns, and the individual poresreach2.585microns.Consequently, high sorption capacityof the anion exchangerOECH-VI-Iapparently due toits surfacea microstructure more precisely and greaterporosity.
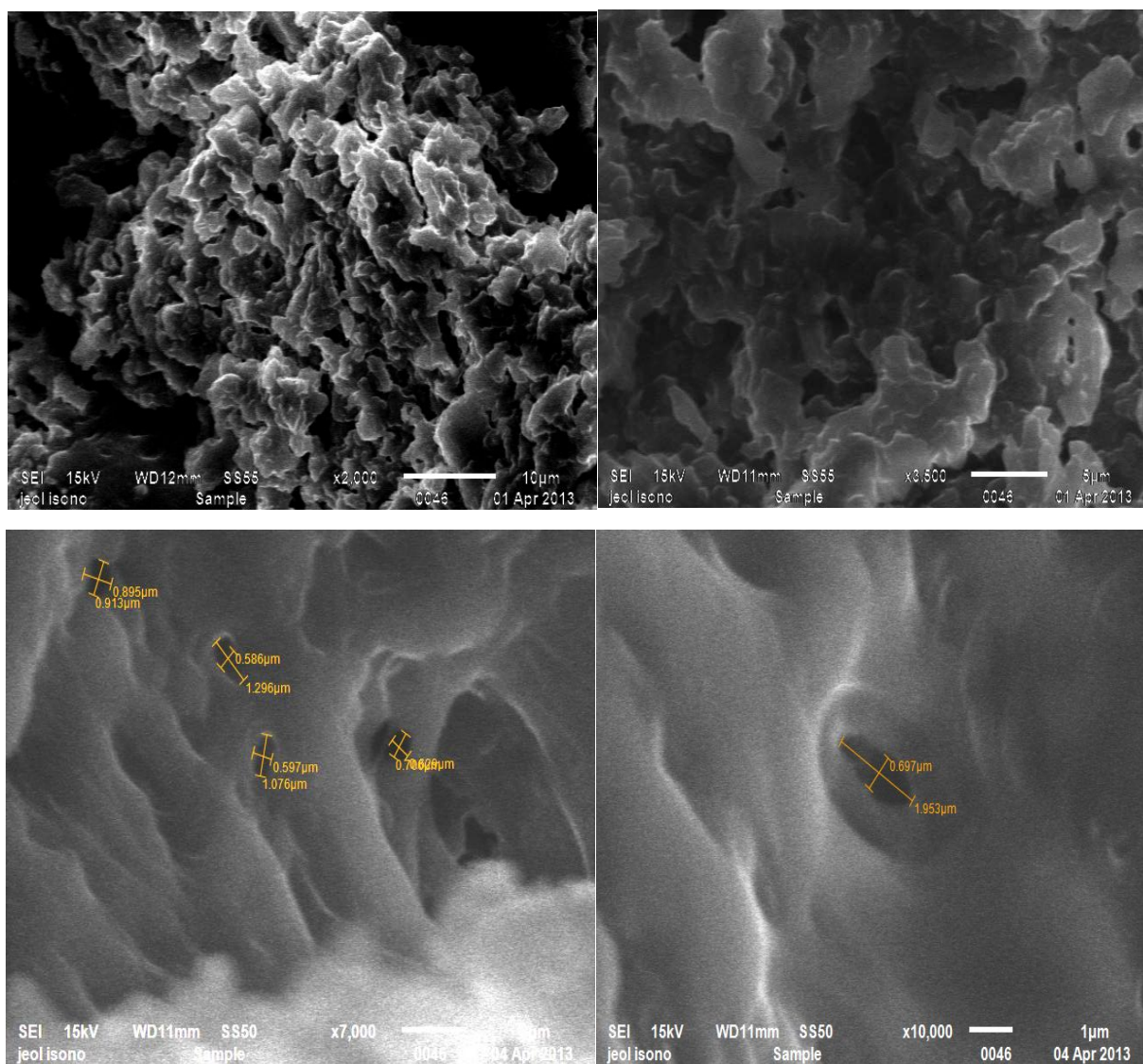
Figure 4 : Microstructuresurface of anion exchangerOECH-VI-I

IV. Conclusion

The sorption activity of new anion exchangers based on oligomers of epichlorohydrin and 4-vinylpyridine towards nickel (II) ions were studied, looking into the dependency on the concentration and pH of the model solutions of Nickel (II) sulfate heptahydrate, and the contact time. It was established that it has a high sorption and good kinetic properties with respect to the nickel (II) ions when extracting nickel (II) from the individual solutions. It was found that at a pH of 5.2 the SC of the ECHO-VP-I anion exchanger reaches maximum values of 346.4 mg /g respectively.

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Determination of Lead Levels in Drinking Water in Some Areas of Khartoum City and Gezira State, Sudan

By Mohammed Mubarek Awad Ahmed & Khalifa Al-Faloos

Asmaria University, Saudi Arabia

Abstract- The present study was designed to examine the concentration of lead in drinking water in Khartoum, Arbagi, Dagala, Wadshantoor, Saleem. Fifty samples of drinking water which collected from different houses in Khartoum, Arbagi, Dagala, Wadshantoor, Saleem and other samples from the Blue Nile for comparison during the period 2013-2014 were analyzed for its lead content by Atomic absorption spectrometry method. Mean lead concentration in samples of drinking water in this study was ranging between 0.012ppm (Blue Nile)-0.046ppm (Khartoum)with a median of 0.02ppm. A positive correlation was found between urbanization and lead mean concentration (0.046ppm) in Khartoum w.r.t (0.025ppm) in Gezira state. So this study recommended that the drinking water delivery system should be free of lead.

Keywords: lead, contamination, drinking water, atomic absorption.

GJSFR-B Classification : FOR Code: 039999

DETERMINATIONOFLEADLEVELSINDRINKINGWATERINSOMEAREASOFKHARTOUMCITYANDGEZIRASTATESUDAN

Strictly as per the compliance and regulations of :

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Mohammed Mubarek Awad Ahmed [α] & Khalifa Al-Faloos [σ]

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I. Introduction

Humans are exposed to lead through inhalation of air pollutants, consumption of contaminated drinking water, exposure to contaminated soils or industrial waste, or consumption of contaminated food. Food sources such as vegetables, grains, fruits, fish and shellfish can become contaminated by accumulating metals from surrounding soil and water. lead exposure causes serious health effects, including reduced growth and development, cancer, organ damage, nervous system damage, and in extreme cases, death. Exposure to heavy metals, such as mercury and lead, may also cause development of autoimmunity, in which a person's immune system attacks its own cells. This can lead to joint diseases such as rheumatoid arthritis, and diseases of the kidneys, circulatory system, and nervous system. (ToxFaQs, 1993).

Lead rarely occurs naturally in water, the natural concentration of lead in surface water has been estimated to be 0.02 μg/liter.(WHO,1987).

Most lead contamination takes place at some point in the water delivery system. This occurs as a result of corrosion, the reaction between the water and lead in parts of the water delivery system. Materials in the water delivery system which may contain lead include service connections, pipes, solder, and brass fixtures.(Chisolm ,2004).

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II. Materials and Methods

a) Drinking water samples

Drinking water samples were collected in Khartoum and some villages of Gezira state (Arbagi, Wadshantoor, Dagala, Saleem) from 30 houses which water supply by metal pipes in Wadshantoor, Dagala, Saleem.Samples from Arbagi where water supply by plastic pipes, a number of samples were collected from the Blue Nile for comparative.Drinking water was sampled in 1.25 liter plastic bottles, the interior of which being previously rinsed three times with sampled water. To preserve the water it was acidified with HNO_3.Table (1) Samples location of drinking water.

Site	Number of Samples	Samples Code
Blue Nile	5	1A
Arbagi	7	2A
Dagala,Wadshantoor, Saleem	18	3A
Khartoum	20	4A
Total	50	

b) Atomic Absorption Spectrophotometer Method

i. Principle of the method

The technique makes use of absorption spectrometry to assess the concentration of an analyte in a sample. It requires standards with known analyte content to establish the relation between the measured absorbance and the analyte concentration and relies therefore on Beer-Lambert law. In short, the electrons of the atoms in the atomizer can be promoted to higher orbitals(excited state) for a short period of time(nanoseconds) by absorbing a definite quantity of energy. This amount of energy is specific to a particular electron transition in a particular element. In general each wavelength corresponds to only one element, and the width of an absorption line is only of the order of a few picometers (pm), which gives the technique its elemental selectivity. The radiation flux without a sample and with a sample in the atomizer is measured using a detector, and the ratio between the two values(the

absorbance) is converted to analyte concentration or mass using the Beer-Lambert law.(A. Walsh ,1955).

ii. *Reagents*

- Mithyl isobutyl ketone(MIBK)
- Diethyldithiocarbamate(DDC): 20g of diethyldithio - carbamic acid- sodium salt were Dissolved in 380 ml of deionized water and filtered through a 0.45-micron Millipore filter. The filtrate was extracted twice with 15ml portions of MIBK.
- Phthalate buffer: 102g of potassium biphthalate were dissolved in 500ml of deionized water, 14ml of 1M HCl were added and diluted to 1 liter with deionized water.
- Hydrochloric acid: HCl concentrated.
- Sodium hydroxide: NaOH 1M. 4g of NaOH were dissolved in 100ml deionized water.

iii. *Standard solutions*

Standard containing 10,25,50,75, and 100μg/literof Pb were prepared (acidified to maintain pH at 1- 2)and treated as described below.

iv. *Sample Preparation*

1. A 200ml aliquot were filtered through a 0.45 micron Millipore filter. The filtrate was acidified with 16 drops of concentrated HCl.
2. 2-100ml of the acidified water sample were transferred into a 250ml Erlenmeyer flask.
3. 3- A 200ml of the phthalate buffer were added and adjusted pH to 3.6.
4. 7ml of the DDC solution were added, transferred to a 500ml separatory funnel, and 15ml MIBK were added.
5. 4- The solution was Shaken vigorously for 30S, allowed phases to separate, and drawn off the MIBK layer into a glass- stoppered test tube.
6. (Perkin- Elmer Co. ,1994)

III. Results and Discussion

Results of the atomic absorption spectrophotometry method about the concentrations of lead in drinking water samples were listedin the tables below:

Table 2 : Quantities of lead in drinking water samples in ppm as determined by the atomic absorption method

No.	Sample Code	Lead Conc.(ppm)	No.	Sample code	Lead Conc.(ppm)
1	1A	0.03	26	3A	0.03
2	1A	0.00	27	3A	0.03
3	1A	0.00	28	3A	0.03
4	1A	0.01	29	3A	0.04
5	1A	0.02	30	3A	0.03
6	2A	0.00	31	4A	0.04
7	2A	0.03	32	4A	0.05
8	2A	0.01	33	4A	0.04
9	2A	0.02	34	4A	0.04
10	2A	0.01	35	4A	0.05
11	2A	0.02	36	4A	0.04
12	2A	0.03	37	4A	0.05
13	3A	0.04	38	4A	0.04
14	3A	0.03	39	4A	0.05
15	3A	0.03	40	4A	0.07
16	3A	0.04	41	4A	0.04
17	3A	0.03	42	4A	0.06
18	3A	0.03	43	4A	0.04
19	3A	0.04	44	4A	0.05
20	3A	0.03	45	4A	0.04
21	3A	0.03	46	4A	0.05
22	3A	0.03	47	4A	0.05

23	3A	0.03	48	4A	0.04
24	3A	0.03	49	4A	0.04
25	3A	0.04	50	4A	0.05

Table 3 : Statistic analysis of concentration of lead in drinking water

Descriptives

Group	N	Mean	Std. Deviation	Std. Error	95% Confidence Interval for Mean		Minimum	Maximum
					Lower Bound	Upper Bound		
Blue Nile	5	0.0120	0.01304	0.00583	0. 0042	0.0282	0.00	0.03
Arbagi	7	0.0171	0.01113	0.00421	0.0069	0.0274	0.00	0.03
Dagala,Saleem,Wadshantoor	18	0.0328	0.00461	0.00109	0.0305	0.0351	0.03	0.04
Khartoum	20	0.0465	0.00813	0.00182	0.0427	0.0503	0.04	0.07
Total	50	0.0340	0.01471	0.00208	0.0298	0.0382	0.00	0.07

Table 4 : Multiple comparison of lead concentration in drinking water between studied groups

Multiple Comparisons

Dependent Variable: pbconc
Tukey HSD

(I) Group	(J) Group	Mean Difference (I-J)	Std. Error	Sig.	95% Confidence Interval	
					Lower Bound	Upper Bound
Blue Nile	Arbagi	-.00514	.00503	.737	-.0185	.0083
	Dagala	-.02022*	.00434	.000	-.0318	-.0087
	Khartoum	-.03450*	.00429	.000	-.0459	-.0231
Arbagi	Blue Nile	.00514	.00503	.737	-.0083	.0185
	Dagala	-.01508*	.00382	.001	-.0253	-.0049
	Khartoum	-.02936*	.00377	.000	-.0394	-.0193
Dagala	Blue Nile	.02022*	.00434	.000	.0087	.0318
	Arbagi	.01508*	.00382	.001	.0049	.0253
	Khartoum	-.01428*	.00279	.000	-.0217	-.0068
Khartoum	Blue Nile	.03450*	.00429	.000	.0231	.0459
	Arbagi	.02936*	.00377	.000	.0193	.0394
	Dagala	.01428*	.00279	.000	.0068	.0217

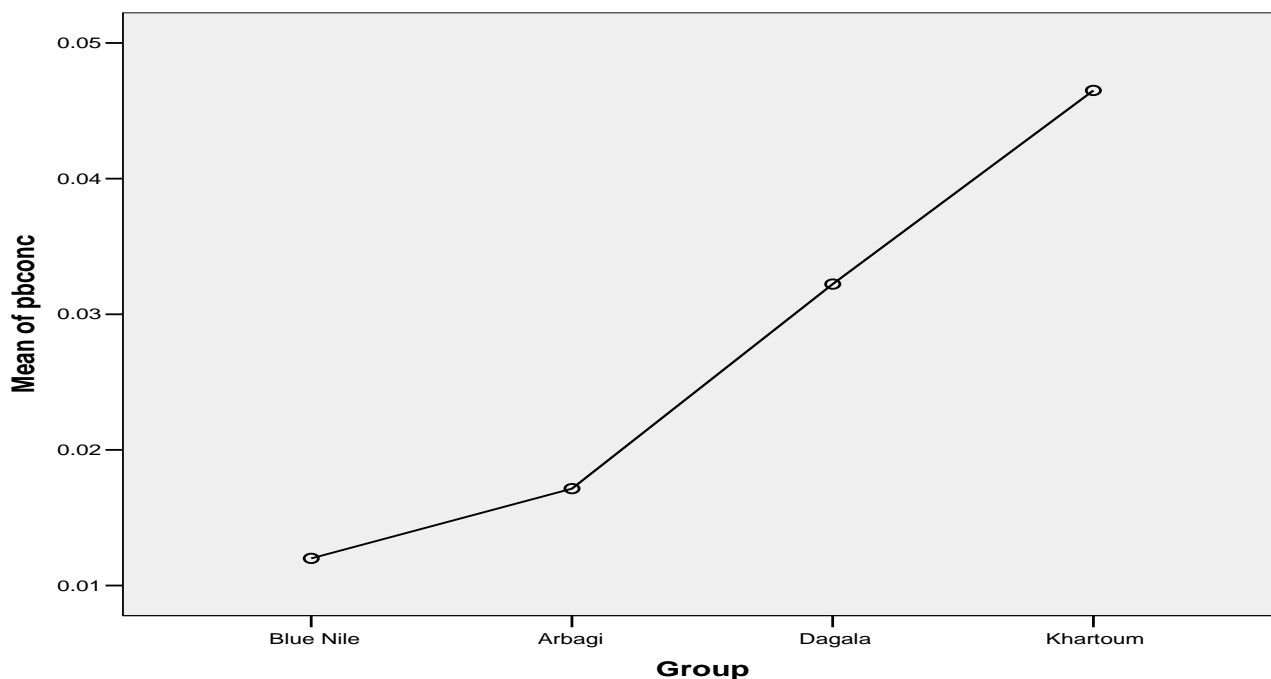*. The mean difference is significant at the .05 level.

Figure 1 : Means of Pb- concentration in the studied groups

Table (2) Summarize data on lead content in drinking water by the atomic absorption method of the studied samples.The concentration of lead was ranged between 0.00-0.07 ppm. The highest concentration of lead(0.07ppm) was found in Khartoum samples and the lowest concentration(0.00ppm) was found in samples of the Blue Nile and Arbagi.Three of the studied samples have zero value. The mean concentration of lead in drinking water by the atomic absorption method was 0.034ppm which was less than the amount allowed by the WHO.

Table(4) shows a multiple comparison of concentration of lead in drinking water between the studied groups.The mean difference was significant at the 0.05 level.

Samples from the Blue Nile was done to make a comparison between the concentration of lead in drinking water before transfer via pipes and after that and this is because most of lead may enter to water should be come from the soldering materials of this pipes. The mean concentration of lead in drinking water of the Blue Nile samples (0.0120ppm) was the lowest value among all other means which prove that much amounts of lead content in water should be come from pipesas expected . Also the results show that the minimum concentration of lead in theBlue Nile samples was 0.00 ppm and the highest concentration of lead in these Samples was 0.03ppm and this concentration was so high with respect to other samples and this is because a lot of lead come to the river from soil and air and from pollutants which were throwed in the river. Samples which were collected from Arbagi where houses that water provided by plastic pipes showed

also low concentrations of lead(average concentration of 0.0171ppm) the lowest concentration in Arbagi samples was 0.00ppm and the highest concentration was 0.03 ppm. The mean concentration of lead in samles from Arbagi(0.017ppm) and samples from the Blue Nile(0.012ppm) were very nearer to each other and that is because there is no soldering materials in pipes that delivered drinking water in Arbagi. Samplesfrom Wadshantoor, Dagala, Saleem where water delivered by metallic pipes have an average value of (0.0322ppm), the lowest lead concentration was 0.03ppm and the highest lead concentration in these villages was 0.04ppm and this is because a lot of lead comes from soldering materials in these metallic pipes. Samples from Khartoum have the mean value (0.0465ppm) which is the highest lead concentration and this is shows that the concentration of lead in drinking water samples of Khartoum were greater than that of the rural areas and this is because that many industries were found in Khartoum and ahuge quantities of industrial wasted which may contain a high concentration of lead should be found there. Also Khartoum was so traffic crowded so the soil and the air of Khartoum would be very contaminated with lead than other rural areas which may affect the concentration of lead in drinking water positively.

The concentration of lead in drinkingwater allowed by the WHO (0.05 ppm) exceeded by only two samples of Khartoum samples (0.07ppm), and (0.06ppm). All other samples of drinking water in the present study were less than the amount allowed by the WHO.

Lead in water may comes from pipe solder, soil, air, and all other environmental pollution,but much lead may come from metal pipes so the concerned authority should try to use plastic pipes in providing drinking water, or use other soldering materials instead of lead.

The mean concentration oflead in water to some extent was not so dangerous (0.034ppm) with respect to the concentration that allowed by the WHO which was 0.05ppm and also the same concentration was allowed by EEC and the USEPA.

Results from this table indicated that there was no significant difference in the concentration of lead in drinking water between the samples that collected from the Blue Nile and the concentration of lead in drinking water of Arbagi where water provided by plastic pipes (sig. 0.737) which means that plastic pipes showed less contamination with lead. Samples of drinking water collected from Dagala, Saleem, and Wadshantoor where water was provided by metallic pipes showed significant difference to that of the Blue Nile (sig.0.00).

Significant difference between the concentration of lead in the drinking water of Arbagi where water provided by plastic pipes and the concentration of lead in drinking water of Dagala, Saleem, and Wadshantour was found (sig.0.001).

The concentration of lead in drinking water from Khartoum showed significant differences to samples collected from all other areas (sig. 0.000)

Fig.(1) presents the range of concentrations of lead in drinking water in the areas under study. And it shows increasing order in the concentration of lead from the Blue Nile, Arbagi, Dagala, and Khartoum.

IV. Conclusion

Atomic Absorption spectrometry method is economical, fairly selective, precise, and more sensitive. The method is free from interferences which is an advantage of this method. Therefore the method can be used for routine analysis of water.

Although children are at greater risk from lead exposure, adult exposures can also result in harmful health effects. Most adult exposures are occupational and occur in lead-related industries such as lead smelting, refining, and manufacturing industries. One frequent source of lead exposure to adults is home renovation that involves scraping, remodeling, or otherwise disturbing lead-based paint. Adults can also be exposed during certain hobbies and activities where lead is used. Workers may inhale lead dust and lead oxide fumes, as well as eat, drink, and smoke in or near contaminated areas.

It should be noticed that all types of contamination may affect each other that means lead from soil may come into water; also lead from air may come into soil, and lead from paint and batteries industry may come into water, soil and air and so on.

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Crystallite Size Dependence on Structural Parameters and Photocatalytic Activity of Microemulsion Mediated Synthesized Zno Nanoparticles Annealed at Different Temperatures

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Abstract- The synthesis of ZnO nanoparticles has attracted considerable interest because of their unique properties and potential applications in a variety of solid state devices, catalytic media etc. By using water-in-oil (w/o) microemulsions, nanodroplets of water were used as chemical reactor to synthesize nanoparticles of zinc oxide. Addition of reducing agent ($(NH_4)_2CO_3$) and zinc salt ($Zn(NO_3)_2$) followed by heat treatment results in the formation of zinc oxide nanoparticles (NPs). The structural and optical properties of the samples were investigated by X-ray diffraction and UV-VIS-NIR absorption spectroscopy. X-ray diffraction revealed the wurtzite structure of ZnO. Percentage of lattice contraction and average particle size of the sample were also calculated from the XRD. Size-dependent blue shifts of absorption spectra revealed the quantum confinement effect. Furthermore, on increasing annealing temperature of ZnO NPs, crystallize size increases which, in turn,decreases the band gap energy and photocatalytic degradation efficiency of phenol.

Keywords: microemulsion, ZnO nanoparticles , size-selective catalysis.

GJSFR-B Classification : FOR Code: 259999p

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Strictly as per the compliance and regulations of :

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J. Sharma [α], M. Vashishtha [σ] & D. O. Shah [ρ]

Abstract- The synthesis of ZnO nanoparticles has attracted considerable interest because of their unique properties and potential applications in a variety of solid state devices, catalytic media etc. By using water-in-oil (w/o) microemulsions, nanodroplets of water were used as chemical reactor to synthesize nanoparticles of zinc oxide. Addition of reducing agent ($(NH_4)_2CO_3$) and zinc salt ($Zn(NO_3)_2$) followed by heat treatment results in the formation of zinc oxide nanoparticles (NPs). The structural and optical properties of the samples were investigated by X-ray diffraction and UV-VIS-NIR absorption spectroscopy. X-ray diffraction revealed the wurtzite structure of ZnO. Percentage of lattice contraction and average particle size of the sample were also calculated from the XRD. Size-dependent blue shifts of absorption spectra revealed the quantum confinement effect. Furthermore, on increasing annealing temperature of ZnO NPs, crystallize size increases which, in turn,decreases the band gap energy and photocatalytic degradation efficiency of phenol.

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I. Introduction

Controlling the size and shape of many metal oxides particles is essential in many advanced applications [1-2]. ZnO, which is a wide band gap semiconductor material with a direct band gap of 3.37eV, is an exceptionally important material for wide applications in areas such as photo catalysis, semiconductors and UV detectors [1-2]. It absorbs ultraviolet (UV) light through a process of electronic excitation between the valence band and conduction band. In conjunction with its high chemical stability and low toxicity, this property of ZnO renders it suitable for use as a UV-screening agent in a diverse range of applications.

Due to its suitable band gap, high thermal stability, non-toxicity, photoactivity and of reasonably low cost, ZnO has been a preferred material for photocatalytic applications. In this respect, it have been utilized traditionally not only to produce useful chemicals [3], but also to convert pollutants in waste streams in innocuous or less harm form [4-6].

ZnO nanomaterials have been synthesized using various methods, including vapor-phase transport [7], chemical vapor deposition [8], magnetron sputtering [9], laser ablation [10], and wet chemical methods [11]. It is conceived that wet chemical routes provide a promising option for the large-scale production of various ZnO nanoparticles. However, these wet chemical methods often face the problem of shape and size control of the products [11].

Compared with the simple solution route, the reverse microemulsion approach, has a special advantage in the synthesis of nanoparticles. Reverse microemulsion is a thermodynamically stable phase separation of water-in-oil aided by a surfactant, where the surfactant shells and water-droplet cores constitute micelles with radii ranging from 5 to 100 nm. The synthesis reaction is confined in the nanodrplets of water, thus the size and shape of the products could be tailored by varying the droplet diameter, whereas the surfactant film can inhibit the aggregation of nanodroplets [11-14].

In this communication, we have attempted to use the microemulsion method for synthesis of ZnO nanoparticles. In this method, initially, small water droplets with a narrow size distribution are formed in a hydrophobic solvent. Then, the reaction takes place in the water droplet, generating zinc oxide nanoparticles with a narrow size distribution. In this paper, we report the effect of annealing temperatures on crystallize size, band gap energy and photocatalytic activity of ZnO nanoparticles.

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II. Experimental

a) Materials and Methods

All the chemical (analytical grade reagents) were purchased from Merck Chemical Reagent Co. Ltd. and used without further purification. To prepare the microemulsion n-octane, CTAB and Pentanol were mixed in weight ratio 5:3:2 by magnetically stirring until the mixture became transparent. The two microemulsion solution containing different reactants were prepared as follows: The microemulsion (ME-1) containing $Zn(NO_3)_2$ reactant was obtained by adding 6 ml of a 0.5M $Zn(NO_3)_2$ aqueous solution to 20ml of oil+ CTAB +Pentanol mixture. Similarly, the microemulsion (ME-2) containing $(NH_4)_2CO_3$ reactant was prepared by adding 5.6 ml of a 0.5M $(NH_4)_2CO_3$ aqueous solution to 20ml oil +CTAB+ Pentanol mixture.

The mixing was done by continuous stirring. ME-1 was added dropwise to the ME-2 under stirring. The mixture of ME-1 and ME-2 was stirred for 6 hours at room temperature. The precipitates was collected by centrifugation at 5000 rpm and washed separately with water and ethanol several times prior to drying in a oven at 80°C until a constant weight was achieved. Finally, the precursor was annealed at different temperatures (400°C to 600°C) for 1 hour. Figure 1 shows the flow chart for the synthesis procedure of ZnO NPs.

b) Characterization

The prepared ZnO nanoparticles were characterized for their phase identification and optical properties. X-ray diffraction pattern for the ZnO NPs was recorded using X-ray diffractometer (Bruker, Advanced D8) with Cu K_α radiation (λ = 1.5418 Å) and Lynx Eye detector to study the crystalline nature, type of phase and the crystallite size in the sample. The sample was scanned in 2θ range of $0° – 90°$ with a scanning rate of $0.02°$ s^{-1}. Crystallite size of each sample (D nm) was determined from the peak of maximum intensity (101) of the phase using Scherrer formula with a shape factor (β) of 0.9 using the XRD line broadening method [15-21]:

$$D = 0.89\lambda/\beta \cos \theta \qquad (1)$$

Where 0.89 is Scherrer's constant, λ is the wavelength of X-rays, θ is the Bragg diffraction angle, and β is the full width at half-maximum (FWHM) of the diffraction peak corresponding to plane and D is the diameter (nm) of a crystallite. The corrected peak breadth was determined by subtracting out the instrumental contribution to the peak breadth from the measured peak width [22].

The inter planar spacing (d) and lattice parameter was evaluated using the relations (2) and (3) :

$$2d \sin\theta = n \lambda \qquad (2)$$

$$1/d^2 = 4/3 (h^2+hk+k^2)/a^2 + l^2/c^2 \qquad (3)$$

Here, θ is the angle of diffraction, λ is the wavelength of x ray, (hkl) are the Miller indices and a, c are the lattice parameters.

The % Interplaner shift in the sample was evaluated using the relation (4):

$$\% \text{ Interplaner shift} = [(\text{standard d} - \text{observed d})/\text{standard d}] \times 100 \qquad (4)$$

The diameter of nanodroplets in microemulsion used in making ZnO NPs was measured by dynamic light scattering using Malvern particle size analyzer and is shown in figure 2. The diameter comes out to be 10.66 nm. These nanodroplets might afford a confined environment for the growth of nanoparticles in the nanometer region. The thermogravimetric analysis was carried out using Mettler Toledo TGA/DTA thermal analyser. The analysis was protected by nitrogen and carried out at a temperature range of 20- 800°C and at a heating rate of 10°C/min.

Morphology of the sample was investigated using scanning electron microscope (SEM with ZEISS). Samples were formed using a suspension of ZnO particles dispersed in distilled water by ultrasonic treatment. A few drops of dilute dispersion were deposited onto a carbon film taped to an aluminium grid and dried in air. The optical transmission/absorption spectra of ZnO were recorded using a UV-VIS-NIR spectrophotometer (Agilent, Carry 5000) in the wavelength range 200- 800 nm.

c) Photocatalytic Activity

Synthesized ZnO NPs were utilized for the photocatalytic degradation of phenol under UV light. In this experiment, phenol was premixed with distilled water to obtain 30 ppm concentration and the study of its photocatalytic degradation was carried out after continuous stirring. Before the degradation processes, 5 ml of 30 ppm phenol solution was mixed with 0.005g of ZnO materials calcined at different temperatures to obtain required solutions of catalyst loading with 1000 ppm concentration. These samples were then allowed to be irradiated under UV light for a fixed time duration in order to observe the effect of ZnO calcined at different temperatures on the degradation processes of Phenol.

After the UV light irradiation for a certain time interval, each sample was centrifuged to separate the suspensions of the ZnO nanoparticles. The concentration of Phenol was measured by UV-VIS-NIR spectrophotometer using Carry 5000 detecter with a scan rate of 120 nm /min in the range of 200 nm to 800 nm. The rate of degradation was studied in terms of changes of the absorption maximum at the absorption peak of 269.75 nm. The photo degradation efficiency of phenol was calculated applying the following equation:

$$\% \text{ Photo degradation efficiency} = C_0 - C/C_0 \times 100 \qquad (5)$$

Where C_0 (in ppm) is the initial phenol concentration ; C (in ppm) is the retained phenol in solution.

III. Results and Discussions

a) Phase Analysis (X-ray diffraction)

X-ray diffraction is a non-destructive and analytical method for identification and quantitative analysis of various crystalline forms of prepared nanoparticles also known as phases present in the samples. The XRD patterns of ZnO nanoparticles calcined at temperatures 400°C, 450°C, 500°C, 550°C and 600°C for 1 hour are shown in figure 3(a)-3(e) respectively. These patterns were recorded by using Bruker D8 Advance diffractometer employing Cu-K$_\alpha$ radiations in the 2θ range 10°- 80°. A definite line broadening of the XRD peaks indicates that the prepared material consist of particles in nanoscale range. From this XRD patterns analysis, we determined peak intensity, position and full-width at half-maximum (FWHM) data.

All strong diffraction peaks are located at (100), (002), (101), (102), (110), (103) and (112) which have been clearly indexed as hexagonal wurtzite phase (JPCDS card number: 05-0664) of ZnO with lattice constants a = 0.324 nm and c = 0.520 nm. The diffraction peaks are sharper with the increase of the annealing temperature, which implies that the crystalline structure tends to more integrity and also the average particle size grows up with increasing annealing temperature as shown in figure 4 and the results are given in Table 1.

From Table 1, It has been observed that change in annealing temperature causes change in crystallize size. This may be due to the fact that, in ZnO nanoparticles, there are a large no of vacancies of oxygen, vacancy clusters, and local lattice disorders present at the interface, which leads to the decrease in the volume of the unit cell. The low temperature annealing can lead to a relaxation in the interface structure, but cannot dispel the local lattice disorders or change the internal structure of the nanograins, so there are no apparent changes in the positions and intensities of XRD peaks. When the annealing temperature increases there is a rapid decrease in the density of vacant lattice sites, vacancy clusters and local lattice disorders and a rapid resumption of lattice parameters and the volume of the unit cell towards normal values, and the grains begin to grow. Hence the particle size increases with increasing annealing temperature [23]. The average particle size, crystallinity and % interplaner shift at different annealing temperature are also tabulated in Table.1

The origin of Lattice contraction is due to the presence of dangling bonds in the surface layer of ZnO nanoparticles. The ions on the surface of ZnO nanoparticles are incompletely coordinated and possess the unpaired electron orbitals. Each of these dangling bonds (Zn^{2+} and O^{2-} ions) forms an electric dipole resulting in a parallel array of dipoles originating in the boundary layer of each nanoparticles lies in this surface and experience a repulsive force. Zno has the property of adsorbing O^{2-} and O^- ions in the surface; hence the repulsive interdipolar force decreases and the attractive electrostatic interaction between Zn^{2+} and O^{2-} increases. Due to this electrostatic attraction, lattice is slightly contracted. The change in % lattice error with calcination temperature is shown in figure 5.

b) SEM Analysis

The SEM is used to produce high-resolution imaging of shapes of substances and to confirm spatial variations in chemical compositions. Figure 6 represents the SEM pictures of ZnO nanoparticles at different annealing temperatures. These pictures confirm the formation of ZnO nanoparticles. These pictures substantiate the approximate spherical shape to the nanoparticles. The SEM of all four samples clearly rectifies the effect of sintering temperature on its surface morphology. The amount of porosity as well as size of pores decreases as sintering temperature is increased. Also the surface gets modified and become smoother for higher annealing temperature. The morphology of nanoparticles reveals that they form nanoclusters at higher temperatures [24-26] i.e. average grain size increased with annealing temperature. This is consistent with XRD results.

c) Band Gap Analysis (UV-VIS-NIR Absorption Spectrum)

The size of the nanoparticles plays an important role in changing the entire properties of materials. Thus, size evolution of semiconducting, nanoparticles becomes very essential to explore the properties of the materials. UV-visible absorption spectroscopy is widely being used technique to examine the optical properties of nanosized particles. Figure 7 shows the UV-visible absorption spectra of ZnO nanoparticles after annealing at different temperatures. The band gap energy was calculated on the basis of maximum absorption spectrum of ZnO nanoparticles according to equation:

$$E_g = 1240 / \lambda \qquad (6)$$

Where E_g is the band gap energy and λ is the lower cut off wavelength (nm) of the nanoparticles [27].

A UV spectrum provides information about optical band gap of the material. The energy band of the material is related to the absorption coefficient α by the Tauc relation (7):

$$\alpha h\upsilon = A (h\upsilon - E_g)^n \qquad (7)$$

Where A is constant, α is the optical absorption coefficient, hυ is photon energy, E_g is band gap and n =1/2 for allowed direct transition. It is clear that the absorption edge shifts to the lower wavelength or higher energy with decreasing size of the nanoparticles. This shift in the absorption edge is due to the quantum size effect. As the annealing temperature increase, the peak

absorption wavelength become red shifted due to decreasing quantum confinement with increasing particle size as shown in figure 8 and the results are given in Table 2.

ZnO nanoparticles did not show clear band gap absorption due to the strong light scattering caused by the large particle size. This might be also due to the aggregation of the particles at higher calcinations temperatures [27-30]

*d) Effect of nanocrystallite size on Photocatalytic Activity*

The UV-vis absorption spectra for photodegradation of phenol using ZnO are presented in figure 9. As can be seen, the photocatalytic efficiency of ZnO decreases with increasing calcination temperature. Decreasing the average particle size increases the number of surface sites available for charge transfer. However, decreasing the particle size also increases the rate of surface charge recombination. For a sufficiently small particle size, surface recombination becomes the dominant process as the charge carriers are formed close to the particle surface and also because the recombination process is faster than interfacial charge transfer [31].

As the annealing temperature increases, photocatalytic degradation of phenol by ZnO NPs decreases due to the formation of larger particle size at higher temperature, thereby reduces the surface area and no. of active sites on the photocatalyst surface, which in turn decrease the no. of Hydroxyl and superoxide radicals. Thus lower degree of degradation [31-34] (Figure 10 &11).

Mechanism of photodegradation of phenol can be explained as follows. When the photocatalyst ZnO is irradiated with ultraviolet (UV) radiation from sunlight or other illuminated light source (e.g. fluorescent lamps), it produces electron–holes pairs on or near the surface (Eq. (8)) through electron transfer from the valence band to the conduction band across the band gap of the semiconductor. This state is referred as the semiconductor's photo-excitation state. The electron–hole pair quickly diffuses to the surface. These photogenerated electron–hole pairs can recombine within a time scale of nanoseconds to radiate heat. Such a short lifetime would not allow the electrons and holes to participate in any chemical reaction.

$$ZnO + h\upsilon \rightarrow ZnO + e_{cb}^{-} + h_{vb}^{+} \qquad (8)$$
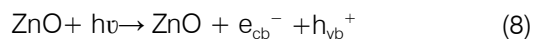
Therefore, the electrons and holes should be captured by any of chemical species which exist on the surface (ions, atoms, molecules, etc.), or by the so-called surface traps. Hydroxyl radicals are generated when the surface adsorbed water or hydroxyl anions react with the valence band hole of the UV excited ZnO (Eqs 9-10).

$$h_{vb} + H_2O \rightarrow \bullet OH + H^{+} \qquad (9)$$

$$h_{vb} + OH^{-} \rightarrow \bullet OH \qquad (10)$$
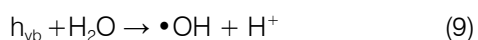
Superoxide radicals are generated by the interaction of atmospheric oxygen or dissolved oxygen of the reaction solution with the conduction band electrons of the UV excited ZnO (Eq.11):

$$O_2 + e_{bc}^{-} \rightarrow \bullet O_2 \qquad (11)$$

These hydroxyl and superoxide radicals attack the adsorbed phenolic compound as long as illumination is continued, or the mineralization of the phenol is completed.

IV. Conclusions

The temperature range of 400 - 600°C was chosen for annealing the sample and to see its effect on crystallize size, band gap and photocatalytic activity. From the above experimental results, following conclusions can be made:

Results of x-ray pattern show that all peaks can be well indexed to the wurtzite phase of ZnO.It also reveal that the lattice slightly contracted due to the presence of dangling bonds on the surface layer of ZnO. In SEM micrographs, the morphology of nanoparticles reveals that they form nanoclusters at higher annealing temperatures i.e. average grain size increased with calcination temperature. This is consistent with XRD results. Absorption peak of the prepared sample is highly blue shifted as compared to the bulk (360nm). Large band gap energy and highly blue shifted absorption edge confirmed that the prepared ZnO nanoparticle exhibit strong quantum confinement effect. As the annealing temperature increases, the particle size of the sample increases. It did not show clear band gap absorption due to the strong light scattering caused by the large particle size. This might be also due to the aggregation of the particles at higher calcinations temperatures.

Photochemical results showed that crystallize size affects the photodegradation. As the particle size increases, the degradation efficiency decreases due to the reduction of the surface area and no. of active sites on the photocatalyst surface, which in turn decrease the no. of Hydroxyl and superoxide radicals.

V. Acknowledgements

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Table 1 : 2θ, % Lattice contraction, Crystallize size & % Crystallinity of (101) plane for ZnO nanoparticle at different annealing temperature

Temperature (ºC)	2 Theta 2θ	Observed d	% Interplaner Shift	Crystallize Size (nm)	Crystallinity %
400	36.323	2.4704	0.19	11.18	86.23
450	36.335	2.4695	0.23	11.66	89.60
500	36.359	2.4680	0.30	14.86	91.20
550	36.444	2.4624	0.52	19.44	93.00
600	36.480	2.4601	0.61	21.28	94.52

Table 2 : Band gap energy, C/C_o & % degradation efficiency for ZnO nanoparticles at different annealing temperatures

Crystallize Size (nm)	Band gap Energy (eV)	C/C_o (For 1 hr)	% Photo degradation efficiency (For 1 hr)
11.18	3.92	0.70	30
11.66	3.83	0.72	28
14.86	3.62	0.76	24
19.44	3.60	0.79	21
21.28	3.51	0.86	14

Table 3 : Lattice parameters and unit cell volume for (101) plane for ZnO nanoparticles at different annealing temperatures

Temperature (ºC)	Lattice parameter (a) (Aº)	Lattice Parameter (c) (Aº)	Unit cell Volume V (Aº)³
400	3.236	5.177	46.94
450	3.235	5.176	46.91
500	3.233	5.173	46.82
550	3.225	5.160	46.48
600	3.222	5.155	46.35
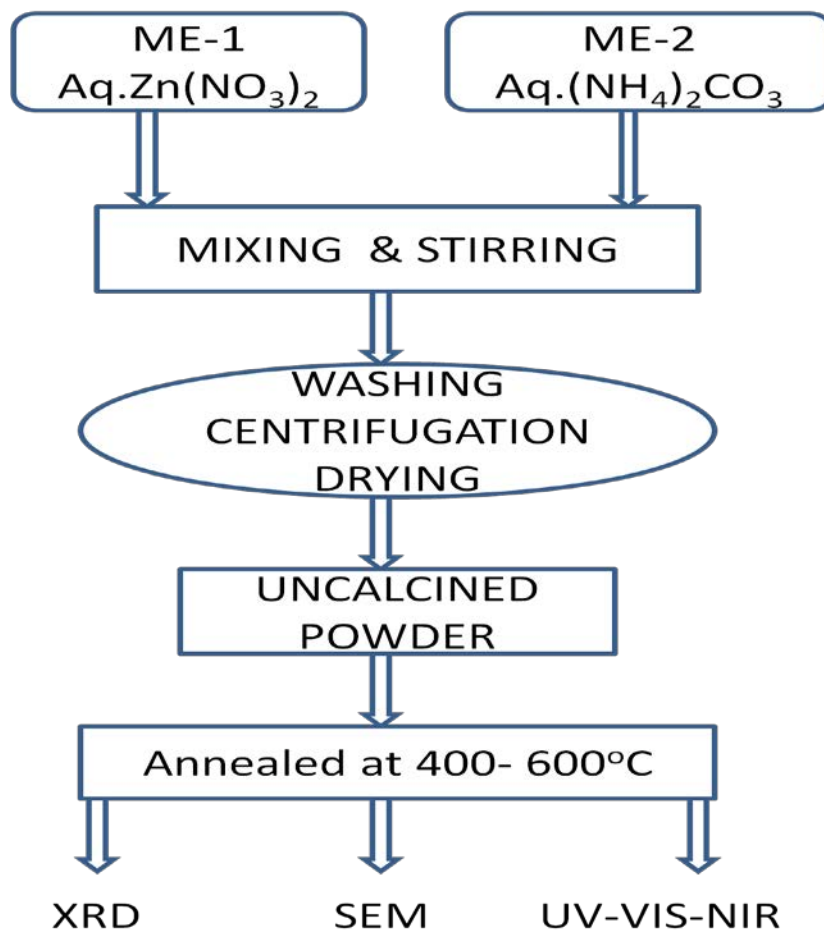
Figure 1 : Flow chart for the synthesis of ZnO nanoparticles by microemulsion method
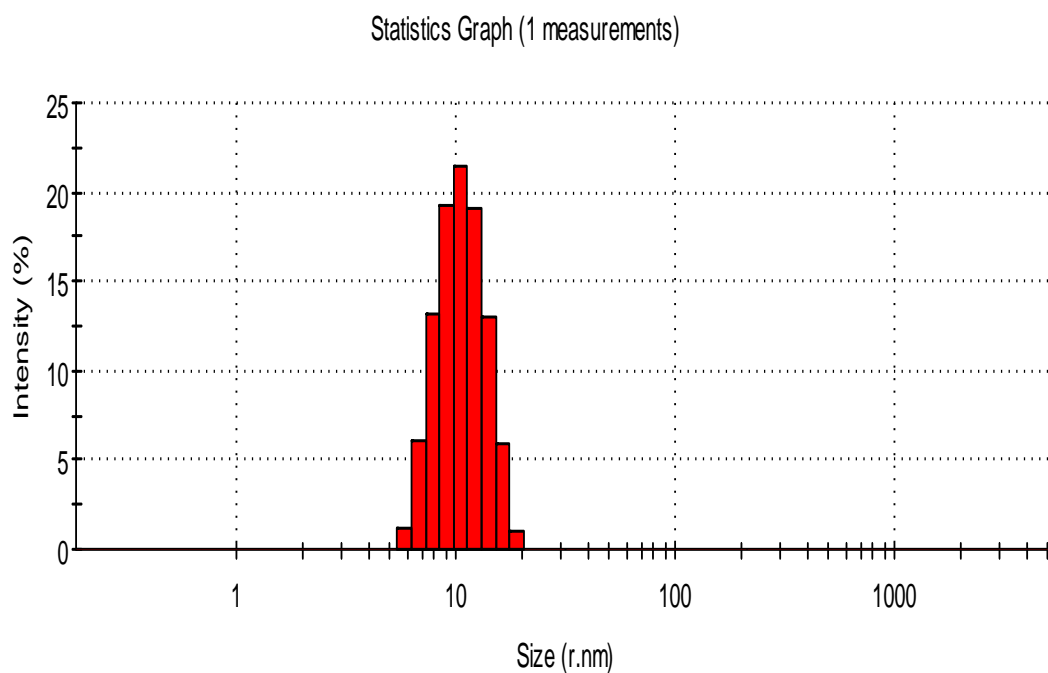
Figure 2 : Core size of microemulsion-1 using particle size analyser
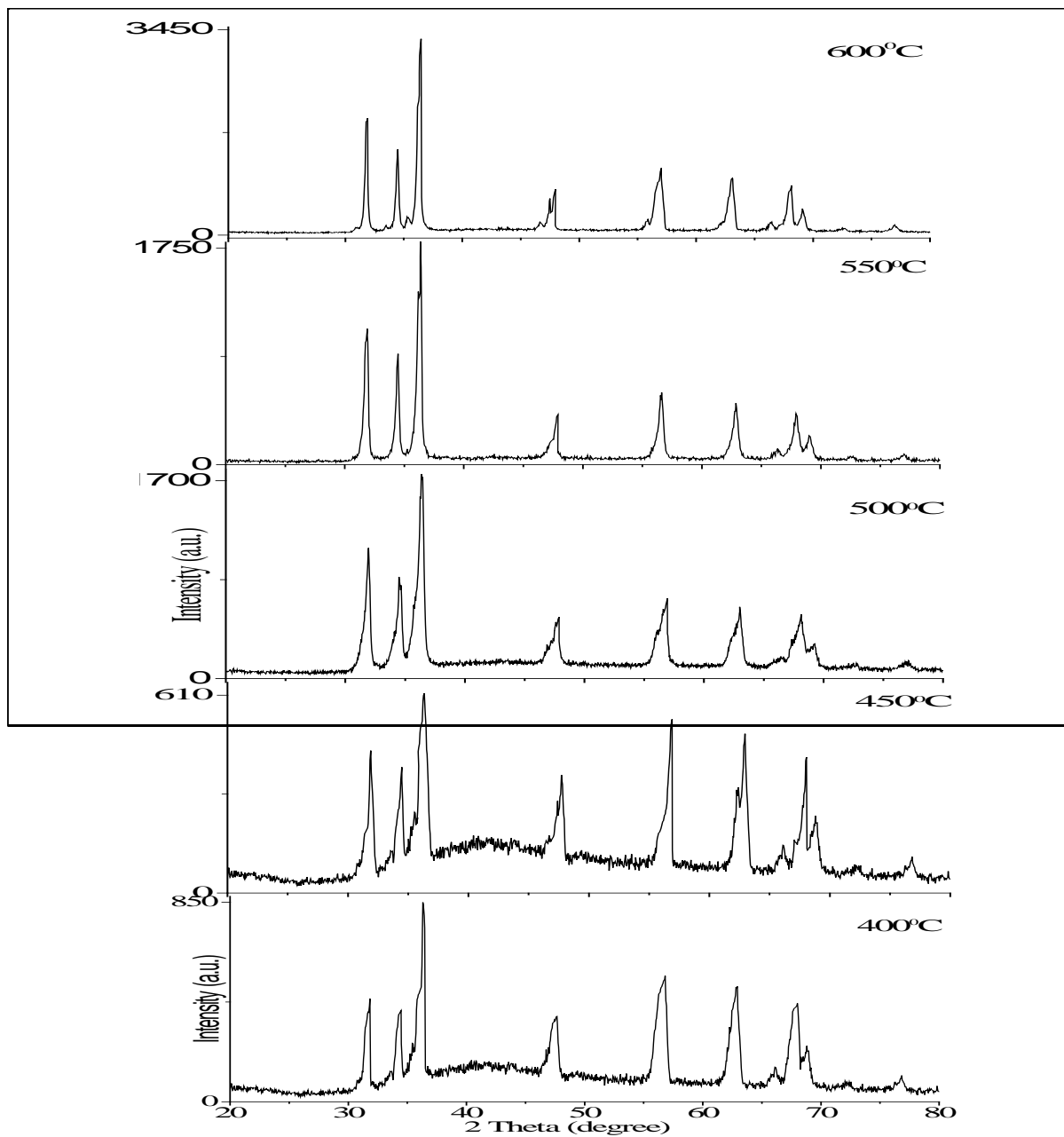
Figure 3 : XRD patterns of ZnO nanoparticles annealed at: (a) 400°C,(b) 450°C,(c) 500°C,(d) 550°C and (e) 600°C
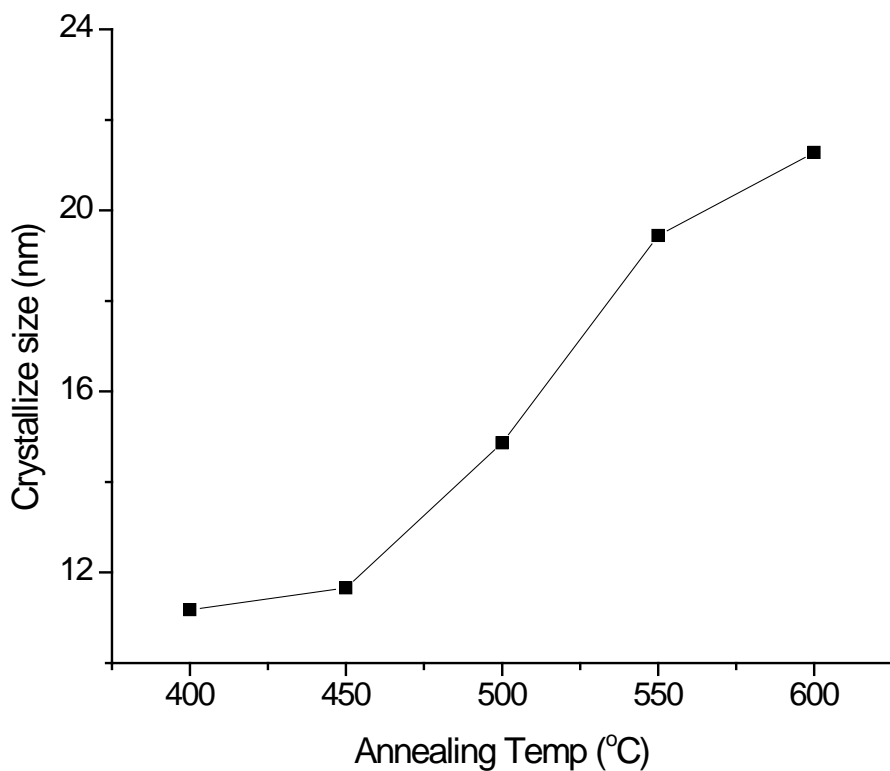
Figure 4 : Crystallize size vs Annealing temperature of ZnO nanoparticles
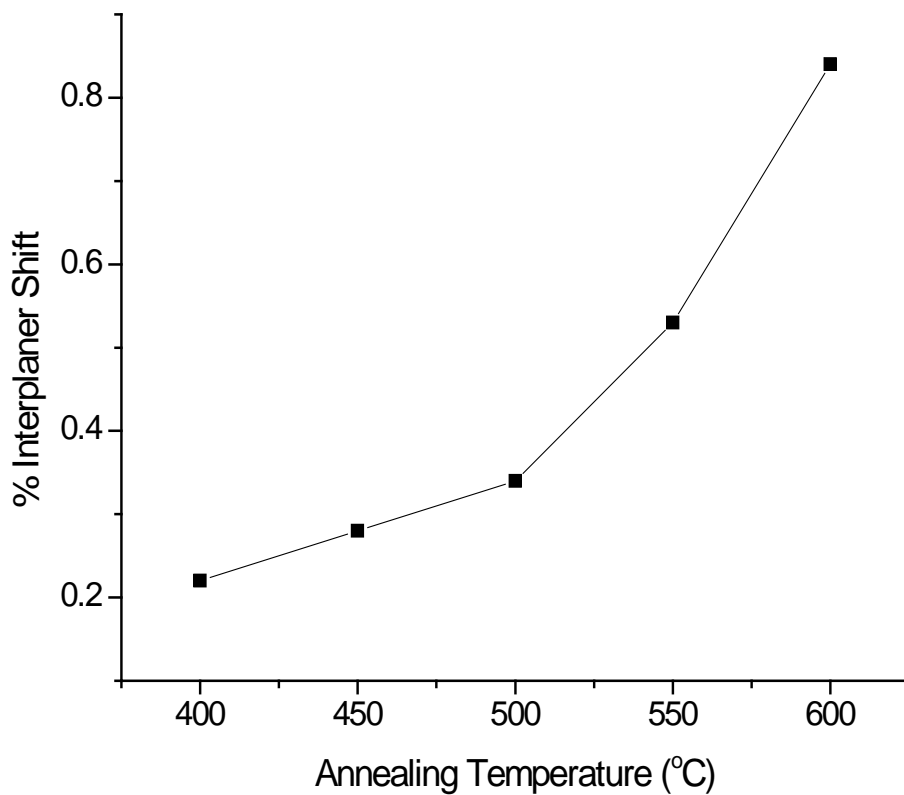
Figure 5 : % Interplaner shift of ZnO NPs at different Annealing temperature
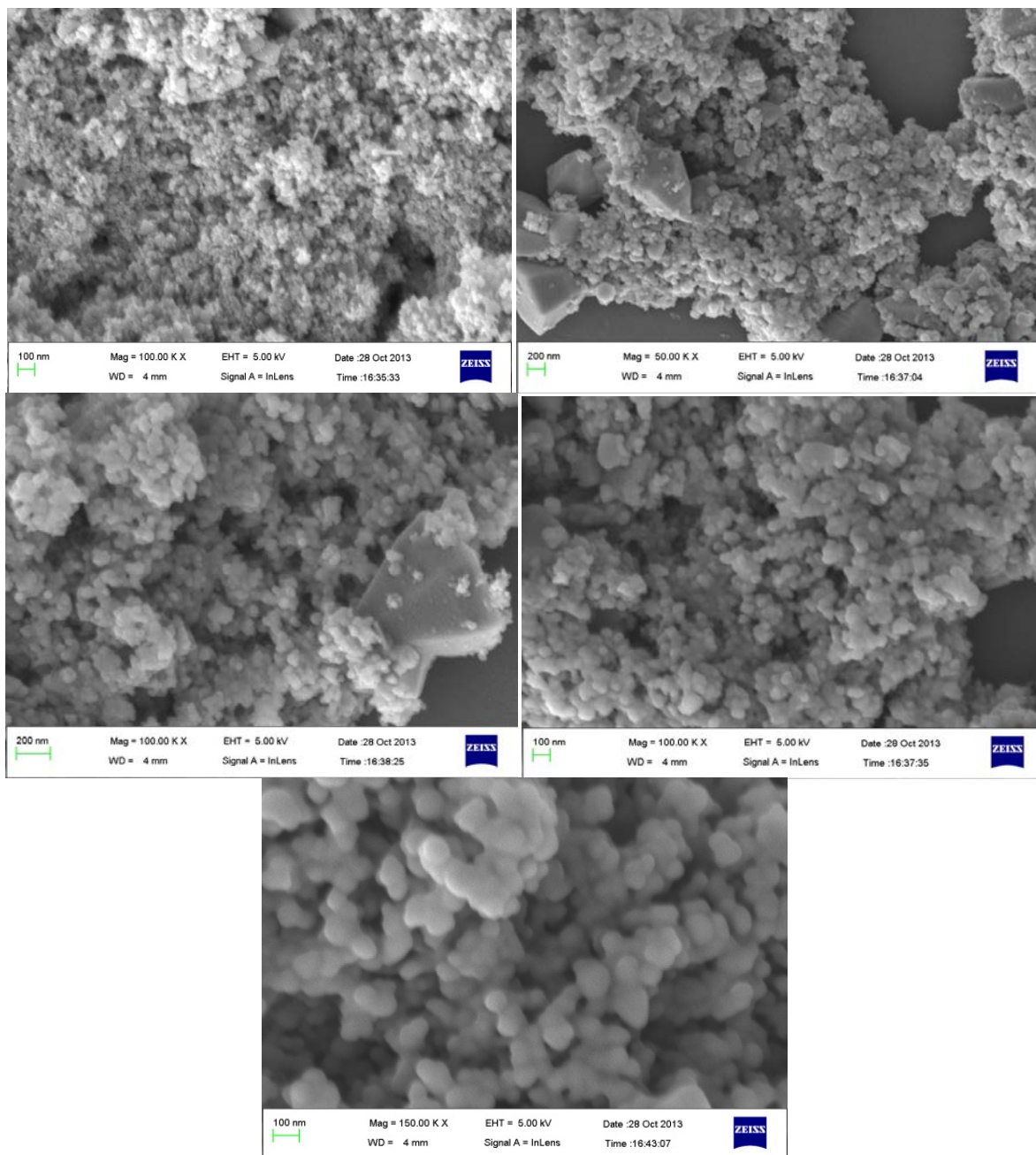
Figure 6 : SEM micrograph of ZnO nanoparticles annealed at (a) 400 (b)450 (c) 500 (d) 550 & (e) 600 °C
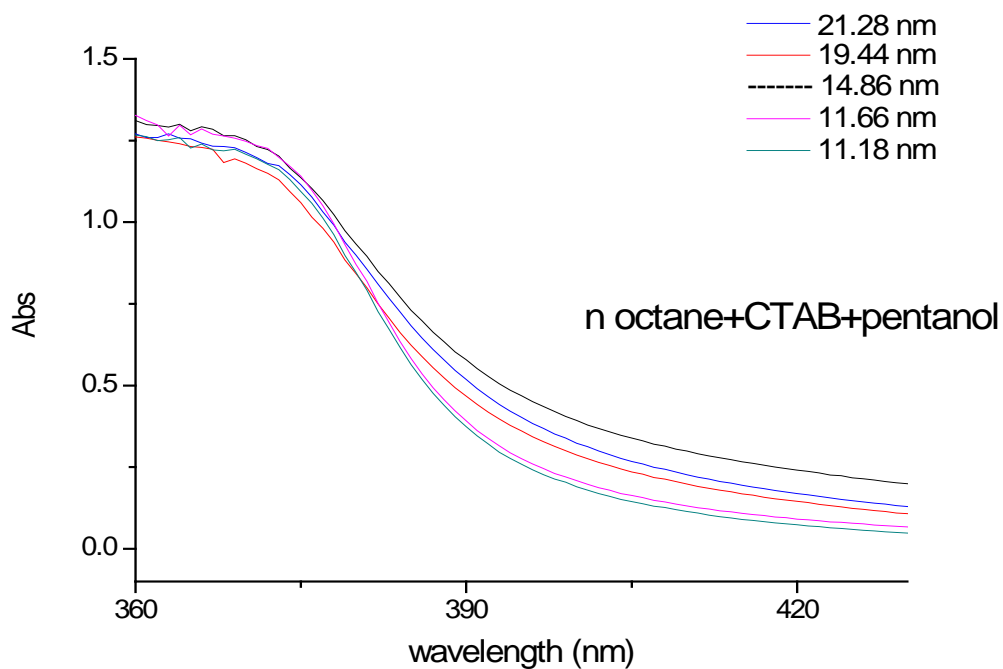
Figure 7 : UV-VIS absorption spectrum of different sized ZnO nanoparticles
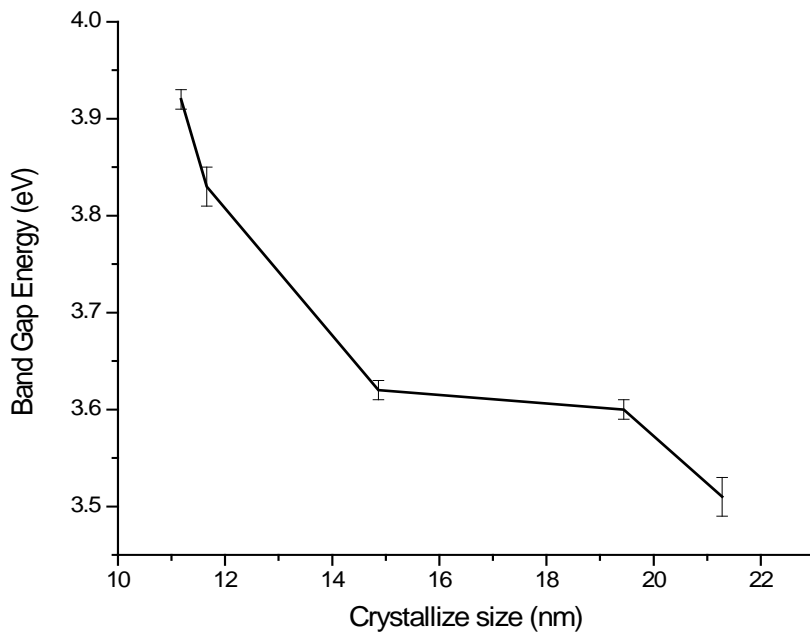
Figure 8 : Crystallize size dependence of band gap energy of ZnO NPs calcined at different temperatures
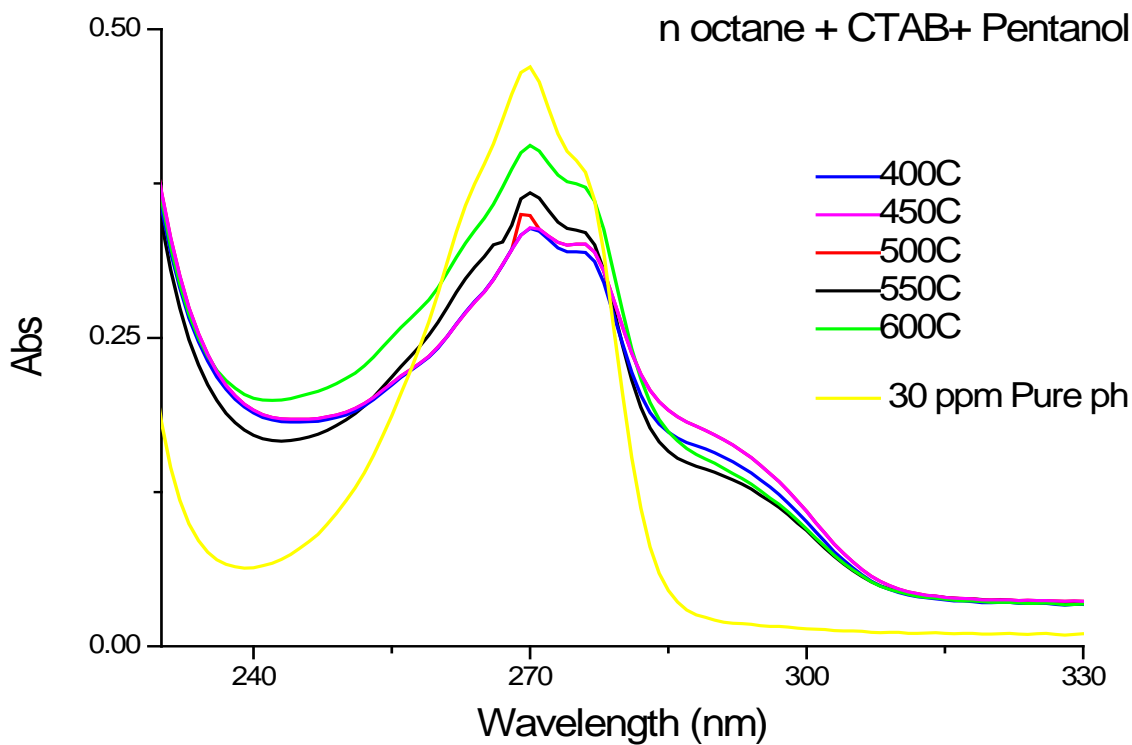
Figure 9 : UV-vis absorption spectra for the degradation of 30 ppm phenol in 1 hour using 1000 ppm ZnO nanoparticles as a catalyst
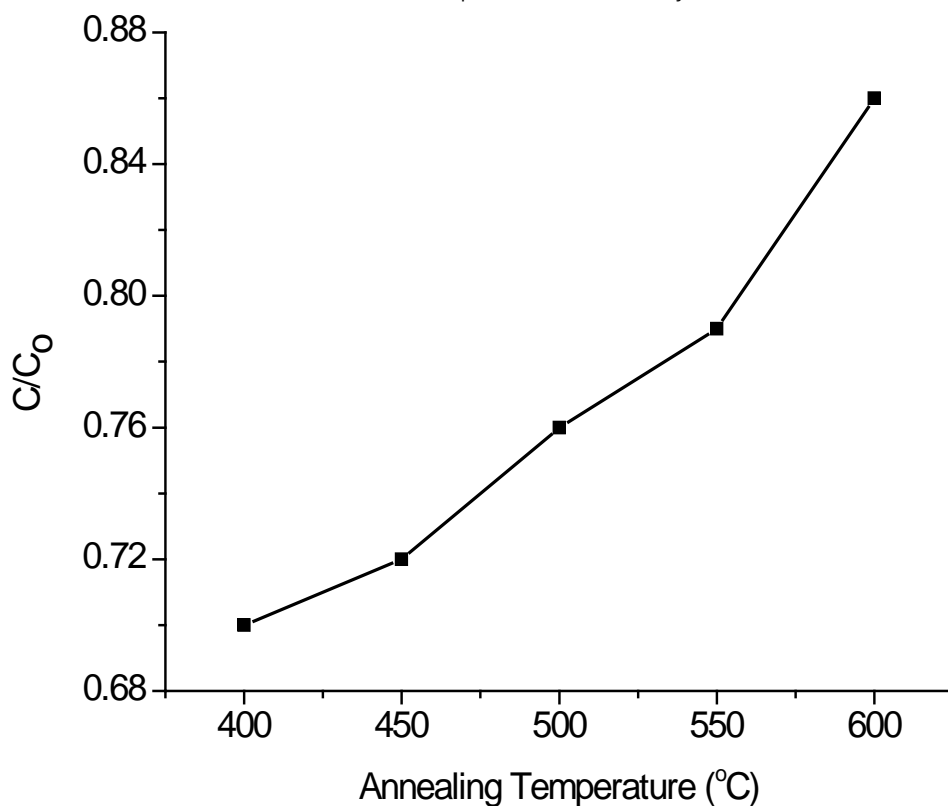
Figure 10 : Plot of C/C_o vs Annealing temperature of ZnO NPs synthesized by microemulsion
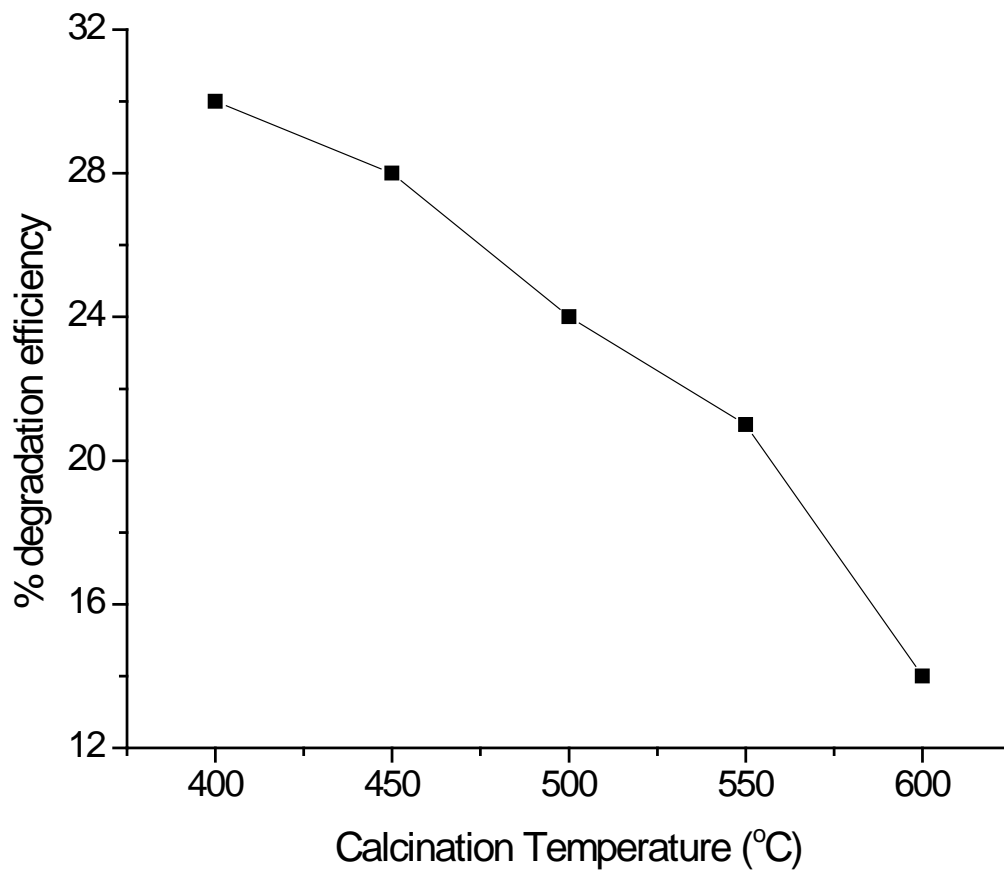
Figure 11 : % degradation efficiency of 30ppm phenol by ZnO NPs annealed at different temperatures

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Synthesis of 1-(2-(4-substitutedphenylamino Imidazo [2,1-B] Benzoxazol-3-yl) Ethanone

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Abstract- 4-acetyl-3-(4-substitutedphenylamino)-isoxazole-5(2H)-one, substituted on nitrogen with a 2-chlorobenzo[d] oxazole group, reacts with triethylamine (TEA) in ethanol under reflux conditions to provide a convenient synthesis of 1-(2-(4-substitutedphenylamino)-imidazo-[2,1-b]-benzoxazol-3-yl)-ethanone.

Keywords: isoxazolones; 2chlorobenzo[d]oxazole; Imidazobenzoxazol; Baseinducedrearrangements.

GJSFR-B Classification : *FOR Code: 259999p*

Strictly as per the compliance and regulations of :

Synthesis of 1-(2-(4-substitutedphenylamino Imidazo [2,1-B] Benzoxazol-3-yl) Ethanone

Chalak Azimi [α], Hatam Maarouf [σ] & Halaleh Ahmadi [ρ]

Abstract- 4-acetyl-3-(4-substitutedphenylamino)-isoxazole-5(2H)-one, substituted on nitrogen with a 2-chlorobenzo[d] oxazole group, reacts with triethylamine (TEA) in ethanol under reflux conditions to provide a convenient synthesis of 1-(2-(4-substitutedphenylamino)-imidazo-[2,1-b]-benzoxazol-3-yl)-ethanone.

Keywords: isoxazolones; 2chlorobenzo[d]oxazole; Imidazobenzoxazol; Baseinducedrearrangements.

I. Introduction

The synthesis of 3-Arylamino isoxazol-5(2H)-one with benzoxazol substituted on nitrogen 1 has been reported[1] by Khalafy and co-workers as shown in Scheme I.

1   X= O   R= H, Br, Me
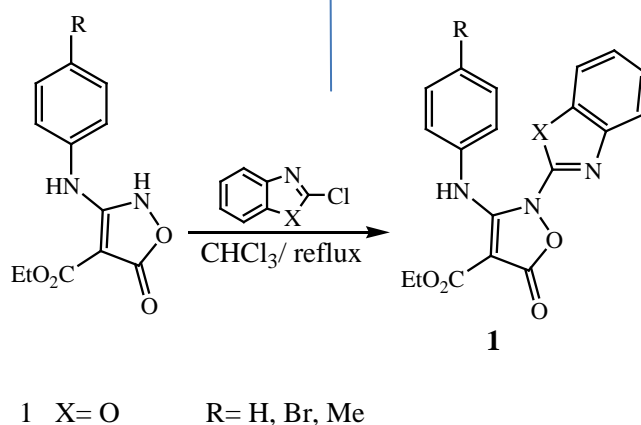
Scheme I

It has been reported[2] that the 2-benzothiazol-2-yl isoxazolones 2 gave the corresponding imidazobenzothiazoles 3 respectively.

2   X= S
R=H, Br, Me, CO$_2$Et, NO$_2$

3   X= S
R=H, Br, Me, CO$_2$Et, NO$_2$
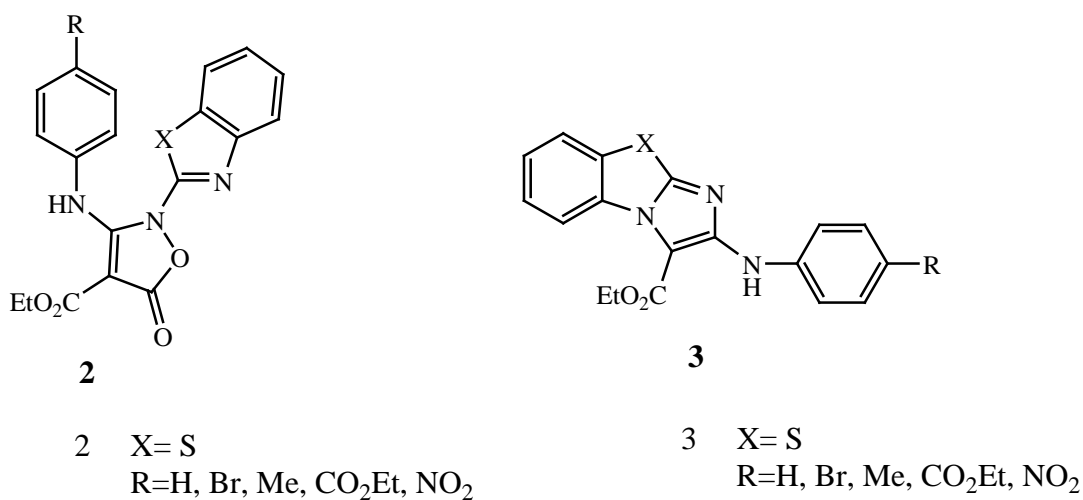
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In previous studies we have shown[3] rearrangement of 4-acetyl-3- (4-substituted phenylamino)- isoxazol-5(2H)-ones substituted on nitrogen with an 2-chloro-5-nitropyridine group (4, R: Br, Me, OMe) to Imidazo [1, 2-a]pyridines (5, R: Br, Me, OMe) under Flash-Vacuum- Pyrolysis(F.V.P) conditions.
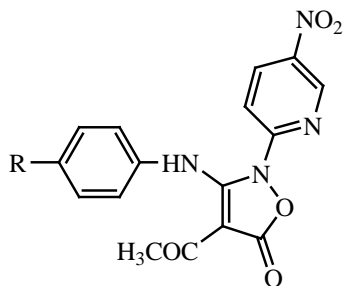
4, R: Br, Me, OMe
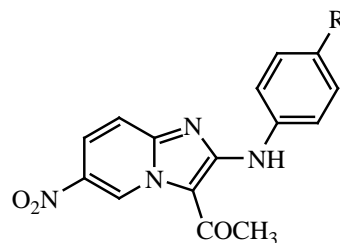
5, R: Br (90%), Me (93%), OMe (95%)

We have also reported[4] synthesis of new N-substituted derivatives of Psubstituted 4 (substitutedphenylamino) isoxazol-5(2H)-ones 6 with a 2-chlorobenzothiazole group substituted on N-2 7, and their rearrangement in the presence of triethylamine to produce 1-(2-(4-substitutedphenylamino)-imidazo[2,1-b] benzothiazole-3-yl) propan-1-one 8, as shown in (Scheme II).

6   **7**   **8**

Et$_3$N
-CO$_2$
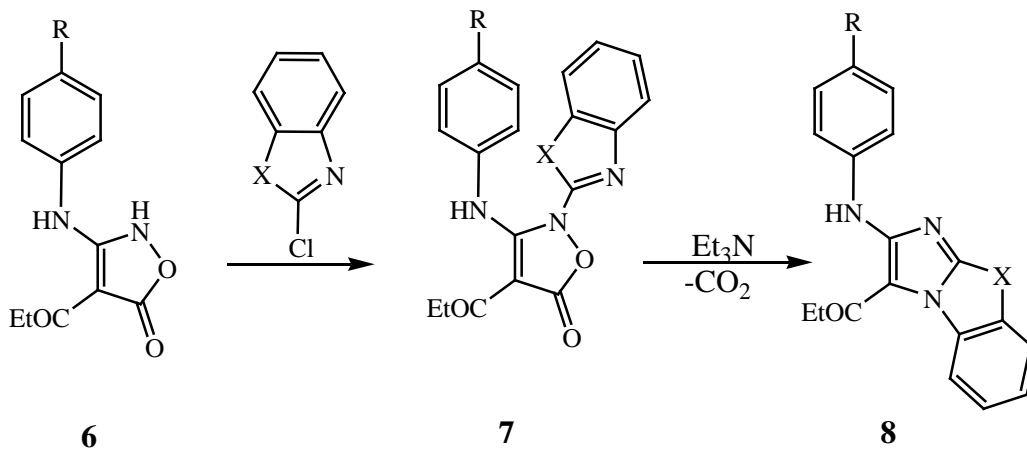
X= S

R= Br, Me, NO$_2$

Scheme II

In this paper we report the synthesis of new N-substituted derivatives of P-substituted 4-acetyl-3-(4-substitutedphenylamino)-5(2H)-one 9 with a 2-chloro benzoxazol group substituted on N-2 10, and their rearrangement in the presence of triethylamine to produce 1-(2-(4-substitutedphenylamino)-imidazo[2,1-b] benzoxazol-3-yl) ethanone 11, as shown in (Scheme III).

9   **10**   **11**

X= O

R= Br, Me, NO_2
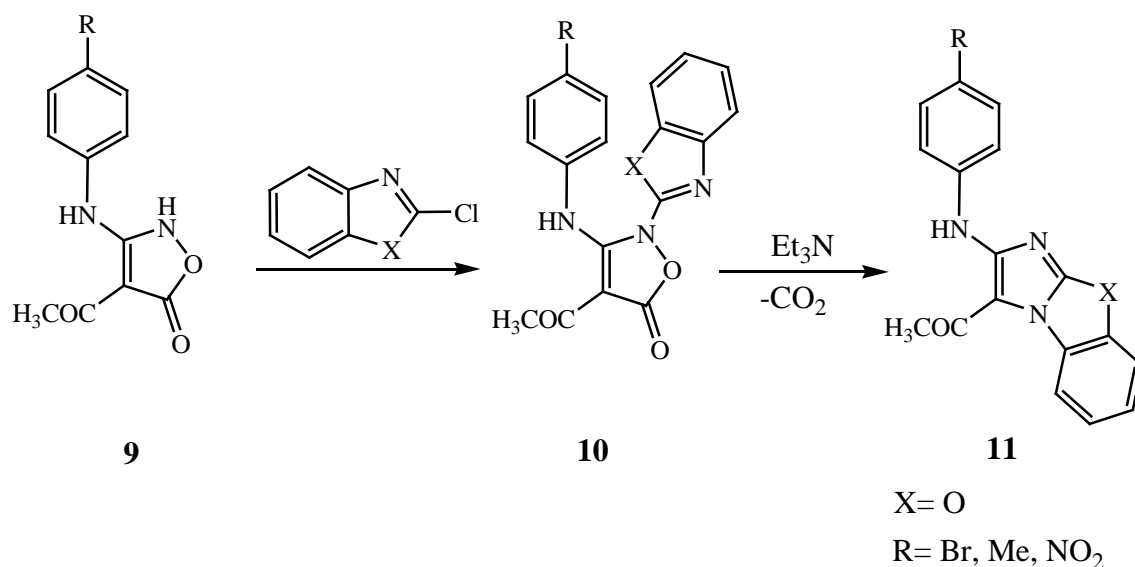
Scheme III

II.   Results and Discussion

    The required isoxazolones 10 were synthesized by reaction of 2-chlorobenzoxazol with 2H-isoxazolones 9, which in turn were made by a modification of the procedure of Worrall.[5,6] Thus, the reaction of the sodium salt of ethylacetoacetate in ethanol with 4-phenylisothiocyanates 12 gave the thiocarbamates 13 in high yield, and these were converted to the corresponding isoxazolone 7 by reaction with 2 equiv of hydroxylamine (Scheme IV).

12   **13**   **9**

R= Br, Me, NO_2
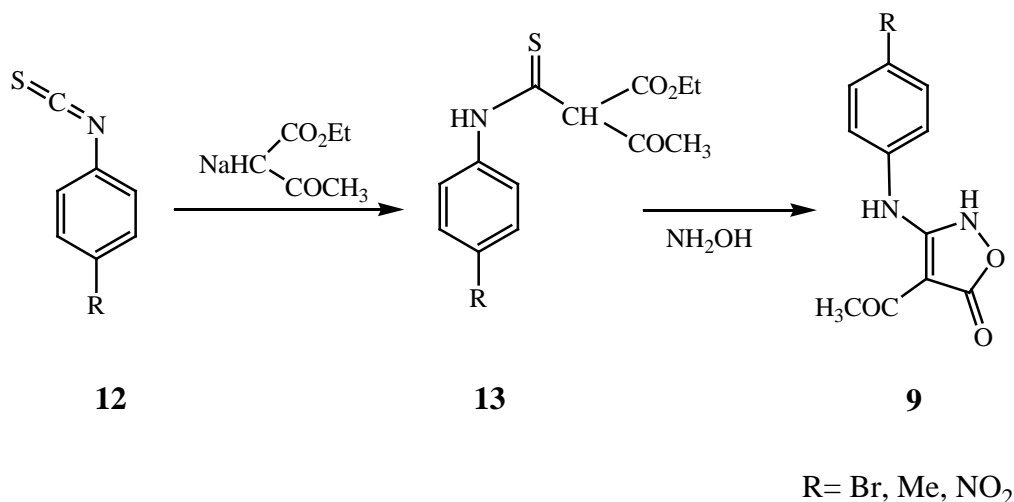
Scheme IV

    N-arylation of 9 with 2-chlorobenzoxazol in toluene under reflux conditions gave the corresponding N-substituted isoxazolones 10 in medium yield. The rearrangement of N-substituted isoxazolones 10, as shown in (Scheme III), proceeded in 45-70% yield in refluxing ethanol for 72 h in the presence of triethylamine (TEA). The reaction pathway leading to the imidazobenzoxazol is consistent with our earlier suggestion for the formation of imidazopyridines, which is consistent with the electronic requirements of the reaction, as shown in (Scheme V), or with the alternative pathway suggested by Prager and co-workers.[7]

10

Et$_3$N

-CO$_2$

11

X= O

R= Br, Me, NO$_2$
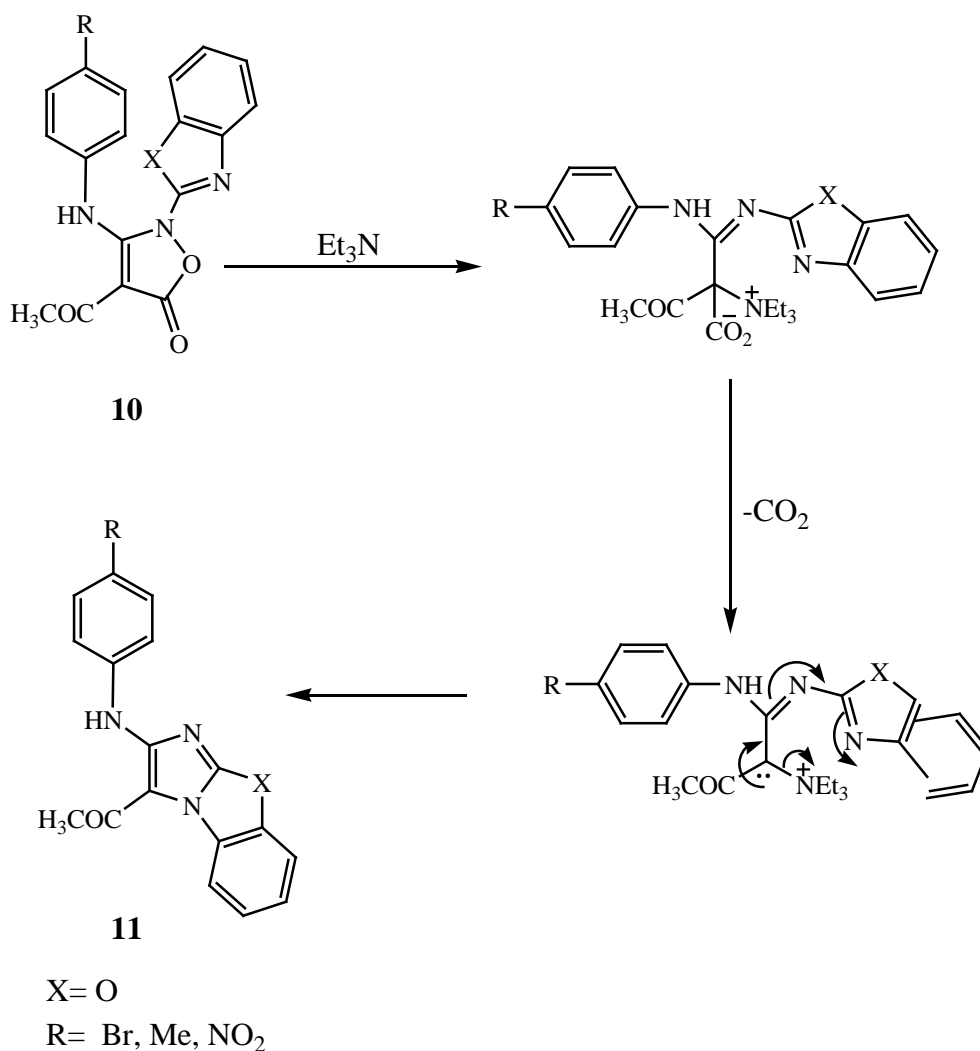
Scheme V

III. Experimental

Freshly distilled solvents were used throughout, and anhydrous solvents were dried according to Perrin and Armarego.[8] Melting points were determined on a Philip Harris C4954718 apparatus and are uncorrected. Infrared spectra were recorded on a Thermonicolet (Nexus 670) FT-infrared spectrometer, using sodium chloride cells and measured as Nujol mulls or KBr. ^{1}H (300 MHz) and ^{13}C (300 MHz) NMR measurements were recorded on a Bruker 300 spectrometer in DMSO-d_6 or CDCl$_3$ using TMS as the internal reference. High resolution mass spectra were recorded on a Varian Matt 311 spectrometer. Mass spectra were registered in a HP 5973 MSD connected to HP 6890 GC interfaced by a Pentium PC and relative abundances of fragments are quoted in parentheses after the m/z values. Microanalyses were performed on a Leco Analyzer 932.

a) *Ethyl-2-((4-bromophenyl)carbamothioyl)-3 oxobutanoate (13, R: Br)*

In a 100 mL round-bottomed flask, absolute ethanol (60 mL) was reacted with sodium (2.9 g, 0.126 mol) and after cooling to room temperature ethylacetoacetate (20 g, 18.90 mL, 0.155 mol) was added. The reaction mixture was stirred at room temperature for 30 min; 4-bromophenyl isothiocyanate (26.82 g, 0.126 mol) was added and the stirring was continued for a further 8 h, during which a yellowish white precipitate of sodium ethyl-2-((4-bromophenyl)carbamothioyl)-3-oxobutanoate salt was formed. The salt was collected and washed with light petroleum ether (b.p. 30-55 $^\circ$C) (4 × 50 mL) to give yellow crystals m.p. 161-167 $^\circ$C (30.14 g, 70%). The pure salt was dissolved in water (50 mL) and neutralized with dropwise addition of HCl (10%) to maintain the pH at 7. The product was extracted with dichloromethane (CH$_2$Cl$_2$) and the extract was washed with water (4 × 50 mL) and dried over anhydrous Na$_2$SO$_4$. Removal of solvent gave (13, R: Br) as a yellow oil (19.8g, 68%). ^{1}H-NMR(CDCl$_3$)(δppm): 1.3 (t, J=7.1Hz, 3H), 2.9 (s, J=7.1Hz, 3H), 4.12 (q, J=7.1Hz, 2H), 5.09 (s, 1H), 7.55 (d, J=8.6Hz, 2H), 7.73 (d, J=8.6Hz, 2H), 10.9 (bs, 1H, NH).

^{13}C-NMR(CDCl$_3$)(δppm): 14.1, 27.8, 63.63, 79.1, 128.37, 132.37, 137.89, 166.08, 188.05.

FT-IR: 3285, 1759, 1723, 1548, 1431, 1285, 1146, 1023, 831 cm^{-1}.

b) *Ethyl-2-((4-methylphenyl) carbamothioyl) -3 oxobuta -noate (13, R: Me)*

This compound was prepared as described above, using 4-methylphenyl isothiocyanate (1.34 g, 9 mmol) and stirring for a further 2 h after addition of 4-methylphenyl isothiocyanate to the ethylacetoacetate salt to give ethyl-2-((4-methylphenyl)carbamothioyl)-3-oxobutanoate (1.92, 71.25%) as pale yellow solid, m.p. 56-59 °C.

^{1}H-NMR(CDCl^3)(δppm): 1.3 (t, J=7.1Hz, 3H), 2.9 (s, J=7.1Hz, 3H), 2.35 (s, J=7.1Hz, 3H), 4.12 (q, J=7.1Hz, 2H), 5.09 (s, 1H), 7.23 (d, J=8.3Hz, 2H), 7.66 (d, J=8.3Hz, 2H), 10.77 (bs, 1H, NH).

^{13}C-NMR(CDCl^3)(δppm): 14.2, 23.57, 27.8, 63.47, 79.2, 126.64, 129.86, 136.41, 166.16, 187.68.

FT-IR : 3284,1760, 1723, 1515, 1430, 1315, 1223, 1148, 1020, 831 cm^{-1}.

c) *Ethyl-2-((4-nitrophenyl)carbamothioyl)-3- oxobuta -noate (13, R: NO2)*

This compound was prepared as described above, using 4-nitrophenyl isothiocyanate (1.62 g, 9 mmol) and stirring for a further 2 h after addition of 4-nitrophenyl isothiocyanate to the ethylacetoacetate salt to give ethyl-2-((4-nitrophenyl)carbamothioyl)-3-oxobutanoate (1.9, 69.25%) as pale yellow solid, m.p. 51-54 °C.

^{1}H-NMR(CDCl^3)(δppm): 1.3 (t, J=7.1Hz, 3H), 2.9 (s, J=7.1Hz, 3H), 4.12 (q, J=7.1Hz, 2H), 5.09 (s, 1H), 6.8 (d, J=8.3Hz, 2H), 7.89 (d, J=8.3Hz, 2H), 10.77 (bs, 1H, NH).

^{13}C-NMR(CDCl^3)(δppm): 14.2, 27.9, 62.47, 79, 123.64, 129.86, 136.41, 143.43, 166.16, 187.68, 199.

FT-IR : 3284,1760, 1723, 1515, 1430, 1350, 1315, 1223, 1148, 1020, 831 cm^{-1}.

d) *4-acetyl-3-(4-bromo phenylamino) isoxazol-5(2H)- ones (9, R: Br).*

To a solution of hydroxylamine hydrochloride (7.06 g, 102 mmol) in water (30 mL), sodium bicarbonate (10.17 g, 102 mmol) was added slowly. Ethanol (80 mL) was added and the resulting potassium chloride was filtered off. Ethyl-2-(4-bromophenyl) carbamothioyl)-3-oxobutanoate (13, R: Br) 12.71g, 34 mmol) was added to the filtrate and the mixture was stirred at room temperature for 24 hours. The reaction mixture was acidified with dilute HCl and the white precipitate was collected and recrystallized from acetone to give the title product (8.78 g, 79%) as colourless needles, m.p: 200-202 °C (dec.);

^{1}H-NMR (D$_6$-DMSO)δ(ppm) 2.25(s, J=7.1Hz, 3H, CH3), 7.37(d, J=8.4Hz, 2H, Ar), 7.57(d, J=8.4Hz, 2H, Ar), 8.30 (bs, 1H, NH), 9.39 (bs, 1H, NH).

^{13}C-NMR (D^6-DMSO)δ(ppm) 15.31, 74.69, 118.02, 125.08, 132.94, 137.10, 163.53, 164.74, 167.39.

FT-IR vmax 3250, 2950, 2740, 1723, 1696, 1666, 1607, 1563, 1456, 1398, 1316, 1183, 1018, 818 cm^{-1}.

e) *4-acetyl-3-(4-methyl phenylamino) isoxazol-5(2H)- ones (9, R: Me)*

This compound was prepared as described above using Ethyl-2-(4-methylphenyl) carbamothioyl)-3-oxobutanoate (13, R: Me) and Refluxing for 24 hours gave colourless crystals (85%), m.p: 164-166 °C (dec.).

^{1}H-NMR (D^6-DMSO+CDCl^3)δ(ppm) 2.30 (s, J=7.0Hz, 3H, CH3), 2.35 (s, 3H, Me), 6.78 (d, J=9.2Hz, 2H, Ar), 6.79 (bs, 1H, NH), 6.80(d, J=9.2Hz, 2H, Ar), 8.85 (bs, 1H, NH).

^{13}C-NMR (D$_6$-DMSO+CDCl$_3$,400 MHz)δ(ppm) 14.52, 20.85, 74.69, 121.53, 130.13, 133.29, 135.64, 163.59, 165.51, 166.74.

FT-IR v$_{max}$ 3669, 2979, 2746, 1705, 1669, 1615, 1331, 1208, 1115, 1023, 800 cm$_{-1}$.

f) *4-acetyl-3-(4-nitrophenylamino)isoxazole-5(2H)- ones (9, R: NO2)*

The compound was prepared as described above using Ethyl-2-(4-nitrophenyl) carbamothioyl)-3-oxobutanoate (13, R: NO2) (1.3 g, 4 mmol) and refluxing for 24 h to give the desired product as colourless crystals (0.5 g,65%), m.p. 162-164 °C.

^{1}H-NMR (d$_6$-DMSO + CDCl$_3$)(δppm): 2.3 (s, J=7.0Hz, 3H, CH3), 6.72 (d, J=9.2Hz, 2H), 6.84(bs, 1H, NH), 7.94 (d, J=9.2Hz, 2H), 8.8 (bs, 1H, NH).

^{13}C-NMR (d$_6$-DMSO+ CDCl$_3$)(δppm): 15.4, 74.69, 118.02, 125.08, 132.94, 137.10, 165.50, 167.74, 171.39.

FT-IR : 3669, 2979, 2746, 1705, 1669, 1615, 1350, 1331, 1208, 1115, 1023, 800 cm^{-1}.

g) *4-acetyl-3-(4-bromophenylamino)-2-(benzoxazol-2- yl)-isoxazol-5(2H)-ones (10, R: Br)*

4-acetyl-3-(4-bromophenylamino)-isoxazole-5(2H)-one (9, R: Br) (116 mg, 0.4mmol) and 2-chlorobenzoxazol (46 mg, 0.3 mmol) were refluxed in toluene (8 mL) for 72 h. The solvent was removed under reduced pressure. On addition of n-hexane (10 mL) to the residue (colourless oil) a white precipitate was formed. The precipitate was filtered and recrystallized from ethanol to give 4-acetyl-3-(4-bromophenylamino)-2-(benzoxazol-2-yl)-isoxazol-5(2H)-ones as white prisms (81.8 mg, 61%) m.p. 156-157 °C.

^{1}H-NMR (d$_6$-DMSO)(δppm): 2.3 (s, J=7.0Hz, 3H, CH$_3$), 6.37(d, J=8.4Hz, 2H), 7.3 (d, J=8.4Hz, 2H), 7.6 (t, J=8.4Hz, 2H), 8.7 (d, J=8.4Hz, 2H), 8.30 (bs, 1H, NH).

^{13}C-NMR (d$_6$-DMSO)(δppm): 26.1, 59.96, 84, 119.02, 124, 126.3, 132.94, 137.10, 163.53, 164.74, 167.39.

FT-IR : 3250, 2950, 2740, 1723, 1696, 1666, 1607, 1563, 1456, 1402, 1398, 1301, 1183, 1018, 818 cm-1.

MS m/z: (%) 413.4 (M+, 12%), 411 (M+, 11%), 405 (82), 397 (71), 371 (48), 369 (40), 334 (25), 294 (28), 291 (27), 290 (100), 262 (30), 224 (27), 177 (33), 161 (34), 150 (40), 135 (26), 134 (33), 108 (29), 44 (65).

h) 4-acetyl-3-(4-methylphenylamino)-2-(benzoxazol-2-yl)-isoxazol-5(2H)-ones (10, R: Me)

This compound was prepared as described above, using the corresponding isoxazolone (9, R: Me) (61 mg, 0.27 mmol) and 2-chlorobenzoxazole (41.3 mg, 0.27 mmol) to give the desired product as white prisms (44 mg, 51%) after recrystalization from ethanol, m.p. 160-163 °C.

^{1}H-NMR (d$_6$-DMSO)(δppm): 2.3 (s, J=7.0Hz, 3H, CH$_3$), 2.35 (s, 3H, Me), 6.37(d, J=8.4Hz, 2H), 7.5 (d, J=8.4Hz, 2H), 7.8 (t, J=8.4Hz, 2H), 8.3 (d, J=8.4Hz, 2H), 8.33 (bs, 1H, NH).

^{13}C-NMR (d$_6$-DMSO)(δppm): 24.3, 26.1, 59.96, 84, 118.02, 121, 125.3, 132.94, 137.10, 163.53, 164.74, 167.39.

FT-IR : 3250, 2950, 2740, 1723, 1696, 1666, 1607, 1563, 1456, 1402, 1398, 1301, 1183, 1018, 818 cm-1.

MS m/z: (%) 349.1 (M+, 12%), 341 (48), 325 (40), 314 (25), 294 (28), 291 (27), 290 (100), 262 (30), 224 (27), 177 (33), 161 (34), 150 (40), 135 (26), 134 (33), 108 (29), 44 (65).

i) 4-acetyl-3-(4-nitrophenylamino)-2-(benzoxazol-2-yl)-isoxazol-5(2H)-ones (10, R: NO2)

This compound was prepared as described above, using the corresponding isoxazolone (9, R: NO2) (89 mg, 0.34 mmol) and 2-chlorobenzoxazole (52.1 mg, 0.34 mmol) to give the desired product as white prisms (43 mg, 49%) after recrystalization from ethanol, m.p. 168 -170 °C.

^{1}H-NMR (d$_6$-DMSO)(δppm):): 2.3 (s, J=7.0Hz, 3H, CH$_3$), 6.7(d, J=8.4Hz, 2H), 7.6 (t, J=8.4Hz, 2H), 7.9 (d, J=8.4Hz, 2H), 8.3 (d, J=8.4Hz, 2H), 8.33 (bs, 1H, NH).

^{13}C-NMR (d$_6$-DMSO)(δppm): 26.1, 59.96, 84, 118.02, 121, 125.3, 132.94, 137.10, 163.53, 164.74, 167.39.

FT-IR : 3250, 2950, 2740, 1723, 1696, 1666, 1607, 1563, 1456, 1450, 1402, 1398, 1301, 1183, 1018, 818 cm-1.

MS m/z: (%) 380.1 (M+, 12%), 372 (48), 356 (40), 334 (25), 294 (28), 291 (27), 290 (100), 262 (30), 224 (27), 177 (33), 161 (34), 150 (40), 135 (26), 134 (33), 108 (29), 44 (65).

j) 1-(2-(4-bromophenylamino)-imidazo-[2,1-b]- benzo-xazol-3-yl)-ethanone (11, R: Br)

The isoxazolone (10, R: Br) (90.2 mg, 0.22 mmol) and triethylamine (0.4 mL) were refluxed in ethanol (10 mL) for 24 hours. The reaction mixture was left to cool to room tempreture and resulting precipitate was colleted to afford 1-(2-(4-bromophenylamino)-imidazo-[2,1-b] benzoxazole-3-yl)-ethanone as white needles (44 mg, 51%), mp 180-184 °C.

^{1}H-NMR (d$_6$-DMSO)(δppm): 2.55 (t, J=7.1Hz, 3H), 6.6(d, J=8.4Hz, 2H), 7.2 (t, J=8.4Hz, 1H), 7.3 (t, J=8.4Hz, 1H), 7.5 (d, J=8.4Hz, 2H), 8.2 (bs, 1H, NH).

13C-NMR (d6-DMSO)(δppm): 26.6, 46, 84, 118.02, 121, 125.3, 132.94, 137.10, 143.53, 144.74, 147.39.

FT-IR : 3250, 2950, 2740, 1723, 1696, 1666, 1607, 1563, 1456, 1450, 1402, 1398, 1301, 1183, 1018, 818 cm-1.

MS m/z: (%) 369.1 (M+, 12%), 357 (48), 340 (40), 334 (25), 298 (28), 295 (27), 293 (100), 262 (30), 224 (27), 179 (33), 161 (34), 153(40), 145 (26), 134 (33), 108 (29), 44 (65).

k) 1-(2-(4-methylphenylamino)-imidazo-[2,1-b]-benzo-xazole-3- -ethanone

The isoxazolone (10, R: Me) (76.7 mg, 0.22 mmol) and triethylamine (0.4 mL) were refluxed in ethanol (10 mL) for 24 hours. The reaction mixture was left to cool to room tempreture and resulting precipitate was colleted to afford 1-(2-(4-methylphenylamino)-imidazo-[2,1-b]-benzothiazole-3-yl)-ethanone as white needles (43 mg, 50%), mp 153 -157 oC.

^{1}H-NMR (d$_6$-DMSO)(δppm): 2.35 (s, J=7.1Hz, 3H), 2.55 (s, J=7.1Hz, 3H), 6.3 (d, J=8.4Hz, 2H), 6.9 (d, J=8.4Hz, 2H), 7.3 (t, J=8.4Hz, 1H), 7.5 (t, J=8.4Hz, 1H), 7.7 (d, J=8.4Hz, 2H), 8.2 (bs, 1H, NH).

^{13}C-NMR (d$_6$-DMSO)(δppm): 24.3, 26.7, 84, 118.02, 121, 125.3, 132.94, 137.10, 143.53, 144.74, 147.39.

FT-IR : 3250, 2950, 2740, 1723, 1696, 1666, 1607, 1563, 1456, 1450, 1402, 1398, 1301, 1183, 1018, 818 cm-1.

MS m/z: (%) 305.11 (M+, 12%), 300 (48), 298 (28), 295 (27), 293 (100), 262 (30), 224 (27), 179 (33), 161 (34), 153(40), 145 (26), 134 (33), 108 (29), 44 (65).

l) 1-(2-(4-nitrophenylamino)-imidazo-[2,1-b]-benzo-xazole-3-yl)-ethanone (11, R: NO2)

The isoxazolone (10, R: NO2) (83.6 mg, 0.22 mmol) and triethylamine (0.4 mL) were refluxed in ethanol (10 mL) for 24 hours. The reaction mixture was left to cool to room tempreture and resulting precipitate was colleted to afford 1-(2-(4-nitrophenylamino)-imidazo [2,1-b]-benzoxazole-3-yl)-ethanone as white needles (40 mg, 47%), mp 199-204 oC.

^{1}H-NMR (d$_6$-DMSO)(δppm): 2.55 (s, J=7.1Hz, 3H), 6.7 (d, J=8.4Hz, 2H), 7.3 (t, J=8.4Hz, 1H), 7.5 (t, J=8.4Hz, 1H), 7.9 (d, J=8.4Hz, 2H), 8.6 (bs, 1H, NH).

^{13}C-NMR (d$_6$-DMSO)(δppm): 26.6, 70.96, 84, 118.02, 121, 125.3, 132.94, 137.10, 143.53, 144.74, 147.39.

FT-IR : 3250, 2950, 2740, 1723, 1696, 1666, 1607, 1563, 1456, 1450, 1402, 1398, 1353, 1301, 1183, 1018, 818 cm-1.

MS *m/z:* (%) 336.11 (M+, 11%), 323 (48), 310 (40), 304 (25), 298 (28), 295 (27), 293 (100), 262 (30), 224 (27), 179 (33), 171 (34), 153(40), 149 (26), 134 (33), 108 (29), 44 (65).

IV. Conclusion

In conclusion we have shown that a variety of N substituted isoxazolones 10, rearranged with Triethylamine to give imidazo-[2, 1-b]-benzoxazole. These rearrangements, therefore, appear to be generally applicable to the synthesis of imidazoheterocycles which are suitable synthetic intermediates for a series of polycyclic heterocycles with possible pharmaceutical applications.

V. Acknowledgments

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Preparation, Characterisation and Reactions of Symmertical and Unsymmetrical Tris(Pentafluorophenyl) Antimony(V) Amides

By Ram Nath Prasad Yadav

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Abstract- Several new symmetrical and unsymmetrical amides of the types $(R_f)_3Sb(NR_2)_2$ and $(R_f)_3RSb(NR_2)$ (where, $R_f = C_6F_5$; $R = C_6H_5$ and $NR_2 =$ -NCOCH$_2$CH$_2$CO, -NCOC$_6$H$_4$CO, -NCOCOC$_6$H$_4$, -NC$_6$H$_4$C$_6$H$_4$, -NNNC$_6$H$_4$, -NC(S)SCH, -NC(CH$_3$Cl)NC$_6$H$_4$, -NC(CH$_3$)NCHCH

have been prepared by the metathesis of $(R_f)_3SbCl_2$ or $(R_f)_2RSbCl$ with the appropriate metal salts of the organic ligands. The amide derivatives were also obtained by the interaction of pentafluorophenylantimony(V) chloride with organic ligand(1:1 &1:2 molar ratio) using triethylamine as hydrogen chloride acceptor. The newly synthesized compounds have been characterized by conventional methods. A tentative trigonal bipyramidal structure is suggested for these compounds. The failure of reaction between $(R_f)_3Sb(NR)_2$ and CS_2 even after prolonged refluxing may be attributed to the weak dipole nature of the CS_2 and the presence of electron withdrawing group on antimony amide.

Keywords: tris(pentafluorophenyl)antimony(v), symmetri -cal, unsymmetrical, metathesis, triethylamine.

GJSFR-B Classification : FOR Code: 030299

PREPARATIONCHARACTERISATIONANDREACTIONSOFSYMMERTICALANDUNSYMMETRICALTRISPENTAFLUOROPHENYLANTIMONYVAMIDES

Strictly as per the compliance and regulations of :

Preparation, Characterisation and Reactions of Symmetrical and Unsymmetrical Tris(Pentafluorophenyl)Antimony(V) Amides

Ram Nath Prasad Yadav

Abstract- Several new symmetrical and unsymmetrical amides of the types $(R_f)_3Sb(NR_2)_2$ and $(R_f)_3RSb(NR_2)$ (where, $R_f = C_6F_5$; $R = C_6H_5$ and $NR_2 =$ -NCOCH$_2$CH$_2$CO, -NCOC$_6$H$_4$CO, -NCOCOC$_6$H$_4$, -NC$_6$H$_4$C$_6$H$_4$, -NNNC$_6$H$_4$, -NC(S)SCH, -NC(CH$_3$Cl)NC$_6$H$_4$, -NC(CH$_3$)NCHCH have been prepared by the metathesis of $(R_f)_3SbCl_2$ or $(R_f)_2RSbCl$ with the appropriate metal salts of the organic ligands. The amide derivatives were also obtained by the interaction of pentafluorophenylantimony(V) chloride with organic ligand(1:1 &1:2 molar ratio) using triethylamine as hydrogen chloride acceptor. The newly synthesized compounds have been characterized by conventional methods. A tentative trigonal bipyramidal structure is suggested for these compounds. The failure of reaction between $(R_f)_3Sb(NR)_2$ and CS_2 even after prolonged refluxing may be attributed to the weak dipole nature of the CS_2 and the presence of electron with drawing group on antimony amide.

Keywords: tris(pentafluorophenyl)antimony(v), symmetri-cal, unsymmetrical, metathesis, triethylamine.

I. Introduction

The literature reveals that the synthesis of reported amido derivatives of antimony could be accomplished via different routes. Reaction of a halogen derivatives with an amine is a common synthetic route employed for the preparation of organoantimony(V) amides derivatives are also available by this method.

$$L = C_5H_{10}NH \qquad (C_5H_{10}NH_2)Cl\ldots\ldots$$ (1)
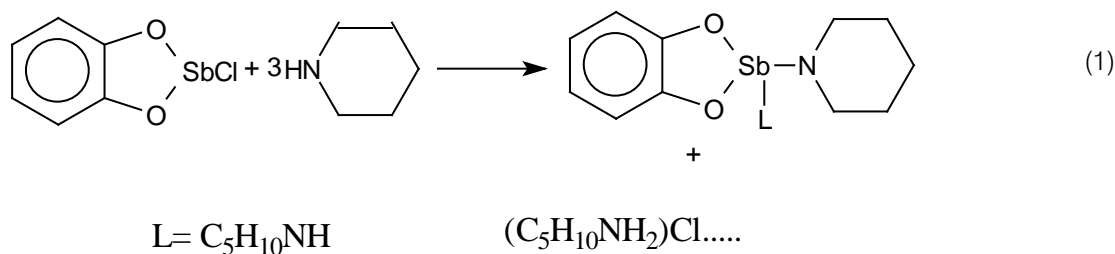
The interaction of triarylantimony dichloride and sodium amide resulted in the formation of triarylantimony(V) imides (Premraj *et al.*1984). These compounds readily give up ammonia to form compounds of higher molecular weight.

Organoantimony(V) amides $(R_3SbCl_2)NH$ (R=Me, Et, Pr, Bu) (Mckenny & Sisler 1967)

$R_3Sb-XNCOYCO$ (R=Me, Ph; X=Cl, Br; Y = $(CH_2)_2$, C_6H_4 (Dahlmann & Winsel 1979) and $(Ph_3SbClNH)_2CO$ have been prepared by the oxidation of $R_3Sb(III)$ with chloroamine, haloamines or N, N-dichloro urea (eqs. 2&3), respectively.
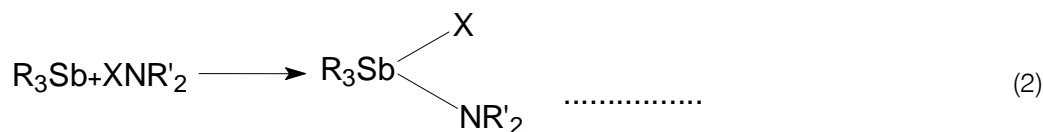
$$[X = Cl, R_2' = H_2; X = Br, R_2' = CH_2COCH_2CO \text{ or } COC_6H_4CO]$$ (2)

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$$R_3Sb + (ClNH_2)_2\,CO \longrightarrow R_3Sb \underset{Cl}{\overset{HN-CO-NH}{\diagdown}} \overset{SbR_3}{\underset{Cl}{\diagup}} \qquad (3)$$
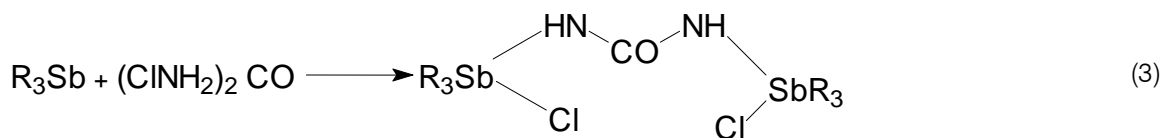
The reaction of triphenylantimony dibromide with silver succinimide proceeded with the formation of triphenylantimony disuccinimide. Both the halogen atoms are readily replaced by two moles of succinide (Bajpai & Srivastava 1979 and Dahlmann & Winsel 1979).The synthesis and biological evaluation of some substituted tertiary arylantimony(V) diamides has been reported by Kiran Singhal et al. (Singhal et al.1987).

The paucity of data on the synthesis and characterization of tris(pentafluorophenyl)antimony(V) diamides and unsymmetric tetraorganostibonium amides, coupled with our interest in the synthesis and reactions of pentafluorophenylantimony(III and V) derivatives (Yadav 2012[a], Yadav 2013[a], Yadav 2013[c] and Yadav 2014) and significant antimicrobial and antitumour activity of pentafluorophenyantimony(V) amides(Yadav 2012[b] and Yadav 2013[b]). With this in mind, we have synthesized a number of symmetrical and unsymmetrical amides of pentafluorophenylantimony(V). The results of these studies are reported in this paper.

II. Result and Discussion

Tris(pentafluorophenyl)antimony(V) diamides and tris(pentafluorophenyl)phenylantimony(V) amides have been prepared by the following two methods.

1. The reaction between pentafluorophenylantimony(V) chlorides and the sodium or silver salt of the corresponding ligands in methanol solvent [eqs. (4) and (5)].
2. The interaction between pentafluorophenylantimony(V) chloride and organic ligand in the mole ratio 1:1 and 1:2 using triethylamine as hydrogen chloride acceptor in methanol solvent [eqs. (6) and (7)].

$$(R_f)_3SbCl_2 + NaNR_2 \xrightarrow{\text{Methanol}} (R_f)_3Sb(NR_2)_2 + 2NaCl\ \dots \qquad (4)$$

$$(R_f)_3R_4SbCl + NaNR_2 \xrightarrow{\text{Methanol}} (Rf)_3RSb(NR_2)\ + NaCl\dots\dots \qquad (5)$$

$$(R_f)_3SbCl_2 + 2HNR_2 + Et_3N \xrightarrow{\text{Methanol}} (R_f)_3Sb(NR_2)_2 + 2Et_3N.HCl\ \dots \qquad (6)$$

$$(R_f)_3RSbCl + HNR_2 + Et_3N \xrightarrow{\text{Methanol}} (R_f)_3RSb(NR_2) + Et_3N.HCl\ \dots \qquad (7)$$

$$R_f = C_6F_5;\ R = C_6H_5$$

$$NR_2 = \overline{NCOCH_2CH_2CO},\ -\overline{NCOC_6H_4CO},\ -\overline{NCOCOC_6H_4},$$

$$-\overline{NC_6H_4C_6H_4},\ -\overline{NNNC_6H_4},\ -\overline{NC(S)SCH},$$

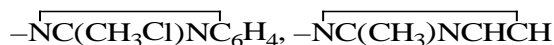$$-\overline{NC(CH_3Cl)NC_6H_4},\ -\overline{NC(CH_3)NCHCH}$$
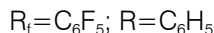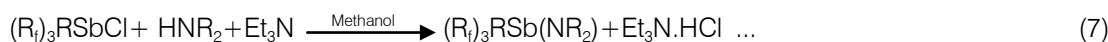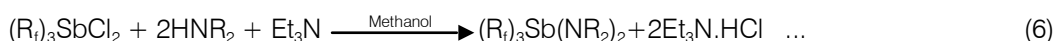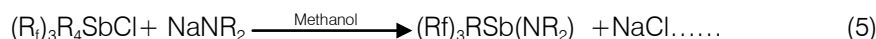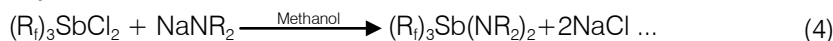
Reactions in both the cases are quite smooth and do not pose any difficulty during work-up. Amido complexes were obtained as dirty white solids and could be crystallized with organic solvent. The melting points of the newly synthesized compounds are sharp. The presence of pentafluorophenyl group imparts not only hydrolytic stability but they could be stored at room temperature, for several weeks. The consistency in melting point of representative compoundsafter 2 or 3 crystallization rules out the possibility of any sort of contamination or side products.

III. Cleavage Reactions

The Sb-N bond in the newly synthesized tris (pentafluorophenyl)antimony(V) diamides, $(R_f)_3Sb(NR_2)_2$ is cleaved in preference to Sb-R_f bond by Br_2 to give corresponding halide.

$$(R_f)_3Sb(\overline{NCOC_6H_4CO})_2 + 2Br_2 \rightarrow (R_f)_3SbBr_2 + 2\overline{COC_6H_4CONBr}\dots\dots\dots(8)$$
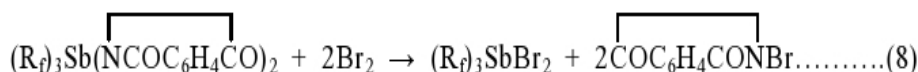
Sb(NMe$_2$)$_5$ is known to react with CS$_2$ to give Sb(SCSNMe$_2$)$_5$. However, $(R_f)_3Sb(NR)_2$ failed to react with an excess of CS$_2$ even after prolonged refluxing on the other hand PhNCO added to the Sb-N bond in the sense of equation shown below.

$$(R_f)_3Sb(NR_2)_2 + 2PhNCO \longrightarrow (R_f)_3Sb(-N-\overset{\displaystyle O}{\overset{\displaystyle \|}{C}}-NR_2)_2 \qquad (9)$$
$$\underset{Ph}{|}$$
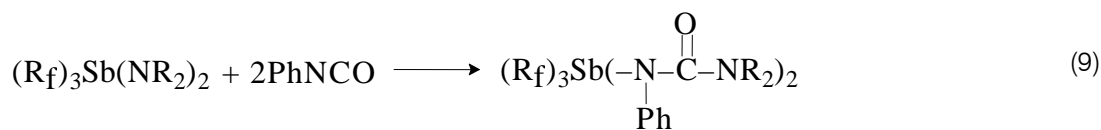
The formation of the PhNCO adduct was confirmed by the absence of NCO at 2200 cm^{-1} and the appearance of a new medium intensity band at 1700 cm^{-1} due to ν(C=O). A medium band 1600 cm^{-1} may be assigned to ν(C-N). The failure of reaction of CS$_2$ with $(R_f)_3Sb(NR_2)_2$ may partly be attributed to the weak dipole nature of the former coupled with the presence of electron with drawing group bonded to antimony amide. Similar course of reactions of CS$_2$, RNCS and RNCO with organometalnitrogen bonded compounds has previously been reported from this laboratory by Premraj *et al.*

IV. Infrared Spectra

Infrared spectra of pentafluorophenylan-timony(V) compounds, $(R_f)_3SbCl_2$ and $(R_f)_3RSbCl$ has been reported earlier from the laboratory (Premraj *et al.* 1985 & Premraj *et al.* 1989). Absorption associated with various mode of vibration of C$_6$F$_5$ group corresponds well with earlier reported values and these do not vary significantly and hence not discussed here.

As has been reported earlier antimony carbon bond corresponding to Y mode for a number of pentafluorophenyl antimony compounds appears in the range of 420-480 cm^{-1}. In the present work the appearance of a band around 460$\pm$5 cm^{-1} can be ascribed to antimony-carbon bond (Nunn *et al.* 1996 and Premraj & Mishra1991).

Assignments of antimony-nitrogen frequencies are quite uncertain due to complicated nature of spectra. An antimony-nitrogen absorption band has earlier been assigned in the range 490-550 cm^{-1}. By analogy, band appearing in the range 500-550 cm^{-1} are tentatively be assigned to terminal ν(Sb-N) vibrations. The comparatively weaker intensity bands located in the region 350-380 cm^{-1} may be due to bridging ν(Sb-N) stretching frequency (Premraj & Mishra 1991).

V. NMR Spectra

The ^{1}H NMR spectra of compound **(1)** $(R_f)_3Sb(\overline{NCOCH_2CH_2CO})_2$ was recorded in CDCl$_3$ using TMS as the reference at 400 MHz instrument. The spectra showed a singlet at δ2.60 ppm (due to –CH$_2$CH$_2$– group) at room temperature suggesting equivalence of both the group.

^{19}F NMR of compound **(1)** was recorded in CDCl$_3$ taking trifluoroacetic acid as internal reference. Signal due to F$_{2,6}$ proton appeared at δ–130.40 ppm while signals due to F$_{3,5}$ and F$_4$ appeared at δ–154.78 ppm and δ–146 ppm respectively.

Thus on the basis of IR,^{1}H NMR and ^{19}F NMR spectra coupled with molecular weight,molar conductance value the newly prepared compounds can be assigned a trigonalbipyramidal structure with three C$_6$F$_5$ groups at equatorial positions and amido groups occupying axial positions.

$$R_f = C_6F_5 \; ; \; NR_2 =$$

-$\overline{NCOCH_2CH_2CO}$, -$\overline{NCOC_6H_4CO}$, -$\overline{NCOCOC_6H_4}$, -$\overline{NC_6H_4C_6H_4}$, -$\overline{NNNC_6H_4}$, -$\overline{NC(S)SCH}$, -$\overline{NC(CH_3Cl)NC_6H_4}$, -$\overline{NC(CH_3)NCHCH}$
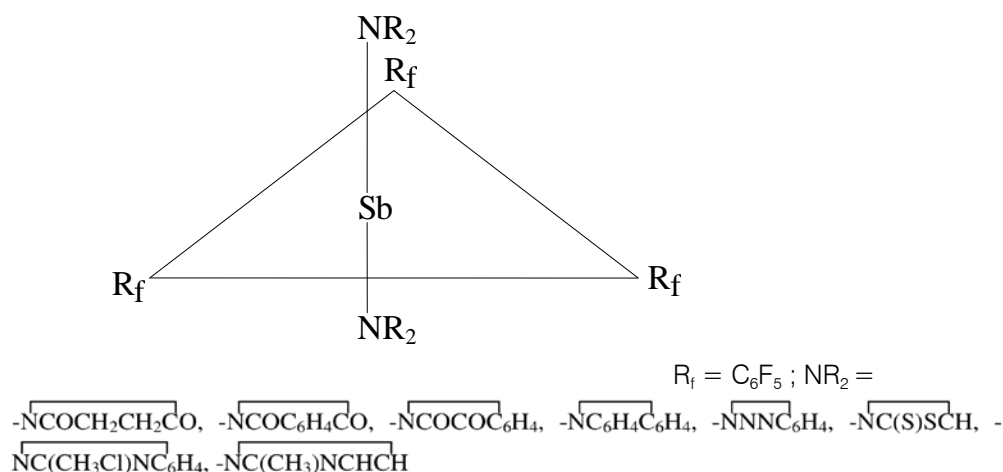
Figure 1 : Suggested structure of $(R_f)_3Sb(NR_2)_2$

VI. Experimental

All solvents were purified, dried and distilled before use as per the literature methods(Vogel 1989).The amides/imide moieties were procured commercially or prepared by the standard techniques and were purified by crystallization. Sodium or silver salts of the organic moieties were freshly synthesized and dried in *vacuo* before use.Tris (pentafluorophenyl) antimony(V) dichloride and tris(pentafluoropenyl) phenylantimony(V) chloride were prepared using reported methods (Premraj *et al.*1985).

IR spectra were recorded in the range 4000-200 cm^{-1} using KBr/CsI pellets on a Perkin-Elmer 577 spectrophotometer.^{1}H NMR spectra were recorded on an EM 360 L Varian spectrometer in CDCl$_3$ containing TMS as an external standard at room temperature. The molar conductance of 10^{-3} M solution was determined at 25°C with a PR-9500 Phillips conductivity assembly. Molecular weights were determined cryoscopically in benzene using a Beckmann thermometer of ±0.01°C accuracy. All reactions were carried out under inert and dry atmosphere. Typical synthetic procedures are given below. Relevant IR assignments, analytical data and molar conductance values are listed in Table 1-4.

a) Reactions of Tris (pentafluorophenyl) antimony(V) Chloride with Succinimide (1)

In an oxygen free atmosphere, a solution of tris(pentaflurophenyl) antimony(V) chloride (0.694g, 1 mmol) in benzene (30 ml) and succinimide (0.198g, 2 mmol) in the same solvent (30 ml) were stirred together in the presence of triethylamine at room temperature for 2h. The reactants were stirred for 1 h more to ensure completion of the reaction. Et$_3$N.HCl (m.p. 248°C) thus formed was filtered off. The filtrate on concentration in *vacuo* yielded a pale yellow crystalline solid and was recrystallized from petroleum ether (40-60°C) to afford tris(pentafluorophenyl)antimony (V) succinimide.M.P.: 145°C ;Yield: 0.524 g (64%).

b) Reaction of Tris (pentafluorophenyl) antimony (V) Chloride with Sodium salt of 2-chloromethyl Benzoimidazole (8)

A solution of tris(pentafluorophenyl)antimony(V) chloride (0.694g,1 mmol) in benzene (30 ml) and sodium salt of 2-chloromethylbenzoimidazole (0.377 g, 1mmol) in the same solvent were stirred together at room temperature for 3 h.NaCl thus formed was filtered off. The filtrate on concentration in *vacuo* afforded a off white crystalline solid and was recrystallized from petroleum ether (40-60°C) to give tris(pentafluorophenyl)antimony (V) 2-chloromethyl benzoimidazole. M.P.: 145°C; Yield: 0.541g, (69%).

c) Reaction of Tris (pentafluorophenyl) phenylantimony (V) Chloride with Carbazole (10)

In an oxygen free atmosphere, a solution of tris(pentafluorophenyl)phenylantimony(V) chloride (0.735g, 1 mmol) in benzene (30 ml) and carbazole (0.167, 1 mmol) in the same solvent (30 ml) were stirred together in the presence of triethylamine at room temperature for 2 h. The reactants were stirred for 1 h more to ensure the completion of the reaction. Et$_3$N.HCl (m.p. 248°C) thus formed was filtered off. The filtrate on concentration in *vacuo* yielded a white crystalline solid and was recrystallized from petroleum ether (40-60°C) to afford tris (pentafluorophenyl) phenylantimony (V) carbazole. M.P.: 170°C; Yield: 0.589 g, (68%).

d) Reaction of Tris (pentafluorophenyl) antimony (V) carbazole with carbon disulphide.

Tris(pentafluorophenyl)antimony(V) carbazole (1.906 g, 2 mmol) was refluxed with an excess of CS$_2$ (2 mmol) for 3 h under nitrogen atmosphere. After removal of volatiles in *vacuo* residue showed no change in the m.pt. or IR spectra as compared to the parent compound.

e) Reaction of Tris (pentafluorophenyl) antimony (V) succinimide with methanol.

Tris(pentafluorophenyl)antimony(V) succinimide was stirred with excess of methanol at room temperature (for 1 h) and then at reflux temperature (for 1 h). After removal of the volatiles the residue showed no change in m.pt. and IR spectra.

f) Reaction of Tris (pentafluorophenyl) antimony(V) isatin with water.

A mixture containing tris (pentafluorophenyl) antimony(V) isatin (1 mmol) and excess of water were refluxed for 3 h. After removal of the solvent, the residue showed no change in the m.pt. and IR spectra.

g) Reaction of Tris (pentafluorophenyl) antimony (V) phthalimide with bromine.

To a solution of Tris (pentafluorophenyl) antimony(V) phthalimide (1 mmol) in CHCl$_3$ (20 ml), bromine (2 mmol) in the same solvent (30 ml) was slowly added at 0°C during 30 minutes. The colour of bromine disappeared immediately after each addition. The mixture was allowed to come at room temperature and then freed from volatiles under *vacuo*. The IR spectra of the residue and TLC in benzene showed the presence of both tris(pentaflurophenyl)antimony(V) bromide and bromophthalimide. No attempts were under made to separate the products.

h) Reaction of Tris (pentafluorophenyl) phenylantimony (V) 2-methylimidazole with phenyl-isocyanate.

A mixture containing equimolar amounts of tris (pentafluorophenyl) phenylantimony(V) 2-methylimidazole (0.781 g, 1 mmol) and phenyl-

isocyanate (0.119 g, 1 mmol) were heated together for 4 h. The resulting brown liquid was treated with petroleumether (60-80º) to afford light browncrystalsof the PhNCO adduct. M.P.: 135°C; Yield: 0.584 g, (65%).

Table 1 : Preparation and Properties of Tris(Pentafluorophenyl) and Phenylantimony(V) Amides

C. No.	Complex $(R_f)_3Sb(NR_2)_2$	Ligand (g)	Recrystallisation solvent	Molar Ratio	M.P. (ºC)	Colour	Yield (g)	Yield (%)
	$R_f = C_6F_5$							
1.	$(R_f)_3Sb(-\overline{NCOCH_2CH_2CO})_2$	$HN\overline{COCH_2CH_2CO}$ (0.198g)	Petroleum-ether (40-60ºC)	1:2	145	Pale yellow	0.524	64
2.	$(R_f)_3Sb(-\overline{NCOC_6H_4CO})_2$	$Na\overline{NCOC_6H_4CO}$ (0.338 g)	Petroleum-ether (40-60ºC)	1:2	190	Off white	0.567	62
3.	$(R_f)_3Sb(-\overline{NCOCOC_6H_4})_2$	$HN\overline{COCOC_6H_4}$ (0.294 g)	Petroleum-ether (40-60ºC)	1:2	200	Off white	0.613	67
4.	$(R_f)_3Sb(-\overline{NC_6H_4C_6H_4})_2$	$Ag\overline{NC_6H_4C_6H_4}$ (0.548g)	Petroleum-ether (40-60ºC)	1:2	210	Light brown	0.659	69
5.	$(R_f)_3Sb(-\overline{NNNC_6H_4})_2$	$HN\overline{NNC_6H_4}$ (0.238 g)	EtOH	1:2	130	Pale yellow	0.498	58
6.	$(R_f)_3Sb(-\overline{NC(S)SCH})_2$	$HN\overline{C(S)SCH}$ (0.334 g)	EtOH	1:2	110	Off white	0.489	59
7.	$(R_f)_3Sb(-\overline{NC(CH_3)NCHCH})_2$	$HN\overline{C(CH_3)NCHCH}$ (0.164g)	CHCl₃	1: 2	205	Off white	0.525	55
8.	$(R_f)_3Sb(-\overline{NC(CH_2Cl)NC_6H_4})_2$	$Na\overline{NC(CH_2Cl)NC_6H_4}$ (0.377g)	EtOH	1:2	145	Off white	0.541	69
9.	$(R_f)_3Sb(-\overline{NCOCH_2CH_2CO})$	$Na\overline{NCOCH_2CH_2CO}$ (0.121g)	Petroleum-ether (40-60ºC)	1: 1	150	White	0.558	70
	$R_f = C_6F_5; Ar = C_6H_5$							
10.	$(R_f)_3ArSb(-\overline{NC_6H_4C_6H_4})$	$HN\overline{C_6H_4C_6H_4}$ (0.167 g)	Petroleum-ether (40-60ºC)	1:1	170	White	0.589	68
11.	$(R_f)_3ArSb(-\overline{NC(S)SCH})$	$Ag\overline{NC(S)SCH}$ (0.274 g)	EtOH	1:1	165	Pale yellow	0.466	58
12.	$(R_f)_3ArSb(-\overline{NC(CH_3)NCHCH})$	$HN\overline{C(CH_3)NCHCH}$ (0.082 g)	CHCl₃	1:1	172	Off white	0.422	54

Table 2 : Elemental Analysis of Tris(Pentafluorophenyl) and Phenylantimony(V) Amides

C. No.	Complex $(R_f)_3Sb(NR_2)_2$	Empirical Formula	Found (Calcd) %		
			C	H	N
	$R_f = C_6F_5$				
1.	$(R_f)_3Sb(-\overline{NCOCH_2CH_2CO})_2$	$C_{26}H_8F_{15}N_2O_4Sb$	37.11 (38.11)	0.97 (0.98)	2.42 (3.42)
2.	$(R_f)_3Sb(-\overline{NCOC_6H_4CO})_2$	$C_{34}H_8F_{15}N_2O_4Sb$	42.60 (44.60)	0.86 (0.88)	2.06 (3.06)
3.	$(R_f)_3Sb(-\overline{NCOCOC_6H_4})_2$	$C_{34}H_8F_{15}N_2O_4Sb$	43.60 (44.60)	0.85 (0.88)	2.00 (3.06)
4.	$(R_f)_3Sb(-\overline{NC_6H_4C_6H_4})_2$	$C_{42}H_{16}F_{15}N_2Sb$	50.75 (52.79)	0.97 (1.68)	1.49 (2.93)
5.	$(R_f)_3Sb(-\overline{NNNC_6H_4})_2$	$C_{30}H_8F_{15}N_6Sb$	39.97 (41.92)	0.89 (0.93)	8.78 (9.78)
6.	$(R_f)_3Sb(-\overline{NC(S)SCH})_2$	$C_{22}H_2F_{15}N_2S_4Sb$	30.74 (31.86)	0.19 (0.24)	2.35 (3.38)
7.	$(R_f)_3Sb(-\overline{NC(CH_3)NCHCH})_2$	$C_{26}H_{10}F_{15}N_4Sb$	37.76 (39.76)	0.99 (1.27)	6.44 (7.14)
8.	$(R_f)_3Sb(-\overline{NC(CH_2Cl)NC_6H_4})_2$	$C_{34}H_{12}F_{15}N_4C_2Sb$	40.78 (42.78)	0.98 (1.26)	4.81 (5.87)
9.	$(R_f)_3Sb(-\overline{NCOCH_2CH_2CO})$	$C_{28}H_9F_{15}NO_2Sb$	41.12 (42.12)	1.00 (1.13)	1.25 (1.75)
	$R_f = C_6F_5 \; ; \; Ar = C_6H_5$				
10.	$(R_f)_3ArSb(-\overline{NC_6H_4C_6H_4})$	$C_{36}H_{13}F_{15}NSb$	48.90 (49.90)	0.99 (1.50)	0.98 (1.62)
11.	$(R_f)_3ArSb(-\overline{NC(S)SCH})$	$C_{26}H_6F_{15}NS_2Sb$	37.87 (38.87)	0.56 (0.75)	0.74 (1.74)
12.	$(R_f)_3ArSb(-\overline{NC(CH_3)NCHCH})$	$C_{28}H_{10}F_{15}N_2Sb$	42.04 (43.04)	0.97 (1.28)	2.59 (3.59)

Table 3 : IR Data of Tris(Pentafluorophenyl) and Phenyl Antimony(V) Amides (Cm^{-1})

C. No.	ν(Sb-C)	ν(Sb-N)^t	ν(Sb-N)^b
1.	425	502	335
2.	435	510	340
3.	440	520	345
4.	438	515	355
5.	450	522	350
6.	460	535	365
7.	455	540	362
8.	475	545	
9.	470	550	370
10.	430	538	376
11.	428	537	373
12.	426	540	380

t = terminal; b = bridging

Table 4 : Molar Conductance [10^{-3}m Solution] and Molecular Weight of Tris(Pentafluorophenyl) and Phen Antimony(V) Amides

C. No.	Molar conductance (Ohm^{-1} cm^2 mol^{-1}) in Acetonitrile	Molecular weight Found (Calcd.)
1.	15.21	1111.25 (818.75)
2.	17.20	1341.22 (914.75)
3.	19.23	1213.29 (914.75)
4.	20.78	1220.84 (945.75)
5.	22.79	1319.25 (858.75)
6.	27.22	1020.25 (828.75)
7.	25.49	1302.45 (953.65)
8.	26.52	1210.25 (784.75)
9.	28.29	1125.25 (797.75)
10.	30.26	1200.30 (865.75)
11.	29.27	1123.65 (802.75)
12.	27.58	1290.50 (780.75)

VII. ACKNOWLEDGEMENT

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Calculation of Proton Range in Some Organic Compounds Energies (1000-100000) keV

By Abothur G. Mohammed, Rashid. A . Kadhum & Dhia. A . Aljouher

Kufa University, Iraq

Abstract- Theoretical study have been done to calculated the Range for protons in ten organic compounds which is: [polypropylene(C_3H_6) ,Polycarbonate ($C_{16}H_{14}O_3$), Mylar ($C_{10}H_8O_4$), Polyvinylalcohol (C_2H_4O), Polyoxymethylene (CH_2O), by using SRIM2013 program written by Mathlab language. the range calculated to protons for energy (1000-100000) keV , by using fitting equations and the semi empirical equation (Devise two equation), and we calculated the rate error and correlation coefficient betweenRange(SRIM) and Range(semi-emp) as seen in tables by using Excel program. The results are agreed with the SRIM 2013 program, so our results showed to be good.

Keywords: proton Range, organic compound.

GJSFR-B Classification : FOR Code: 030599

CALCULATIONOFPROTONRANGEINSOMEORGANICCOMPOUNDSENERGIES1000100000KEV

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Calculation of Proton Range in Some Organic Compounds Energies (1000-100000) keV

Abothur. G. Mohammed [α], Rashid. A. Kadhum [σ] & Dhia. A. Aljouher [ρ]

Abstract- Theoretical study have been done to calculated the Range for protons in ten organic compounds which is: [polypropylene(C_3H_6) ,Polycarbonate ($C_{16}H_{14}O_3$), Mylar ($C_{10}H_8O_4$), Polyvinylalcohol (C_2H_4O), Polyoxymethylene (CH_2O), by using SRIM2013 program written by Mathlab language. the range calculated to protons for energy (1000-100000) keV , by using fitting equations and the semi empirical equation (Devise two equation), and we calculated the rate error and correlation coefficient betweenRange(SRIM) and Range(semi-emp) as seen in tables by using Excel program. The results are agreed with the SRIM 2013 program, so our results showed to be good.

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I. INTRODUCTION

Niels Bohr published a seminar paper on the theory of charged particle penetration in matter, based solely on classical physics. Bohr's early work is instructive because for the first time a unified theory of stopping was attempted [1]. He evaluated the classical stopping of a fast heavy charged particle to an electron bound in a harmonic potential [2]. Consider a charge particle entering into a medium with kinetic energy. Then the average value of the distances that a particle travels before coming to rest, is called the "Range". The range of a proton in an absorbing medium will be somewhat smaller than the path length as measured from the original angle of incidence into the material, because the proton will undergo multiple coulomb scattering [3]. The charged particles when passing in the material medium losing part of its kinetic energy at any collision operation with the target matter as it is known. The continuous of this operation on the particle path in the medium causing decreasing kinetic energy for charged particles until reaching to zero, its losing all the kinetic energy and reaching to the rest state in the certain point. So the total range for charged particles passing in the material medium can be define as the length path that the particle passing before reaching to the rest , and depending on the matter target and the type of the incident particle in addition to its energy [4]. Range- energy relations for protons have been obtained by several authors, such as Livingston and Bethe, Sternheiner, Bichsel, etc. Sternheimer has carried out calculations [5], to determine range energy relations for some of the commonly used materials

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Aluminum, copper, Carbon, Beryllium and lead for proton energy from 2 MeV to 100GeV. Bichsel has also obtained range energy relation for the same substances from 1MeV to 100MeV [6].

In similar fashion, empirical range relations have been developed for other charged particles. The proton is range in air [7]:

$$R_{air} = \left(\frac{E_p}{9.3}\right)^{1.8} \tag{1}$$

Where Ep is the proton energy< 200 MeV.

Bichsel has measured the range of protons in aluminum, and his results can be presented by [8]:

$$R_{Al} = \begin{cases} 14.21E^{1.5874} & 1MeV < E_P \le 2.7MeV \\ \frac{10.5E_P^2}{0.68+0.434\ln(E_P)} & 2.7MeV < E_P \le 20MeV \end{cases} \tag{2}$$

The range in the compound is given by [9]:

$$R_{com} = \frac{M_{com}}{\sum_i n_i (\frac{A_i}{R_i})} \tag{3}$$

II. RESULTS AND DISCUSSION

We have done the calculation range of protons for ten organic compounds with energies (1000-100000) keV and by using a program written with Mathlab.

a) Fitting equation

By using the SRIM_2013 program, which have been written in the Mathlab_2011 program and by using coincidence tool (curve fitting tool), we achieved to find an equation (4) with its Constants (a, b) it is shown in the table (1) and (2) in any medium of ten organic compounds. Which represent the range equations of protons.

$$R(E) = aE^b \tag{4}$$

Where R is the Range; E is the kinetic energy of proton. Its unit meter.

b) Semi Empirical formula for protons range

We got a semi empirical formula for ten compounds by substitution the energy, Atomic number and ionization potential

$$R = \frac{E^{1.75} * \log Z_2^X}{2.1875*10^{9.5} (\log I)} \tag{5}$$

The unit of R is m
R is the range
E is the energy of proton

Z is atomic number of target
I is ionization potential of target
X is the variable

$$x = \begin{cases} 1.05 \text{ at} & (16 \leq Z2 \leq 46) \\ 0.84 \text{ at} & (47 \leq Z2 \leq 65) \\ 0.78 \text{ at} & (66 \leq Z2 \leq 195) \\ 0.66 \text{ at} & (195 \leq Z2 \leq 350) \end{cases}$$

Through the semi empirical formula we got results agreement with the program SRIM 2013. From these figures (1), (2), (3), (4)(5), (6), (7), (8), (9), and (10) we concluded that the results are very good.

Figure 1 : shows the relationship between the range and energy of compound C3H6 was the correlation coefficient (0.99998) and the error ratio(0.000263)

Figure 2 : shows the relationship between the range and energy of compound C16H14O3 was the correlation coefficient (0.999912) and the error ratio(0.000201)

Figure 3 : shows the relationship between the range and energy of compound C10H8O4 was the correlation coefficient (0.999917) and the error ratio(0.000172)
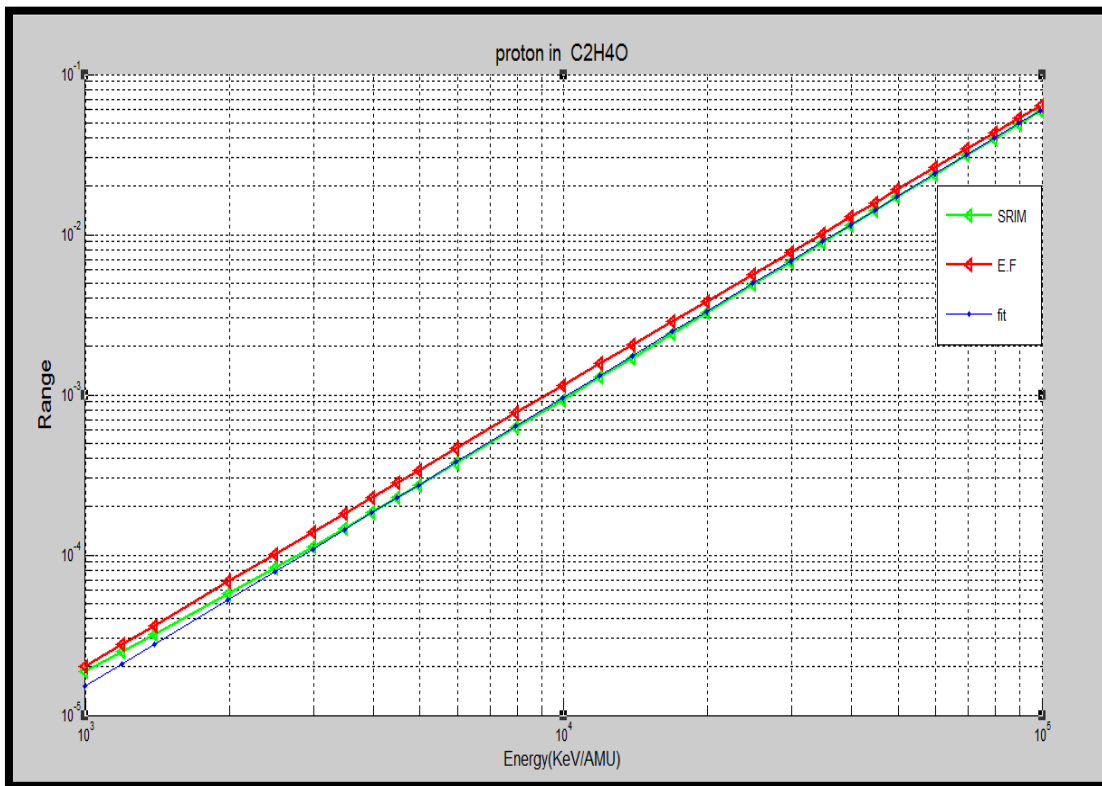
Figure 4 : shows the relationship between the range and energy of compound C2H4O was the correlation coefficient (0.999909) and the error ratio(0.000182)

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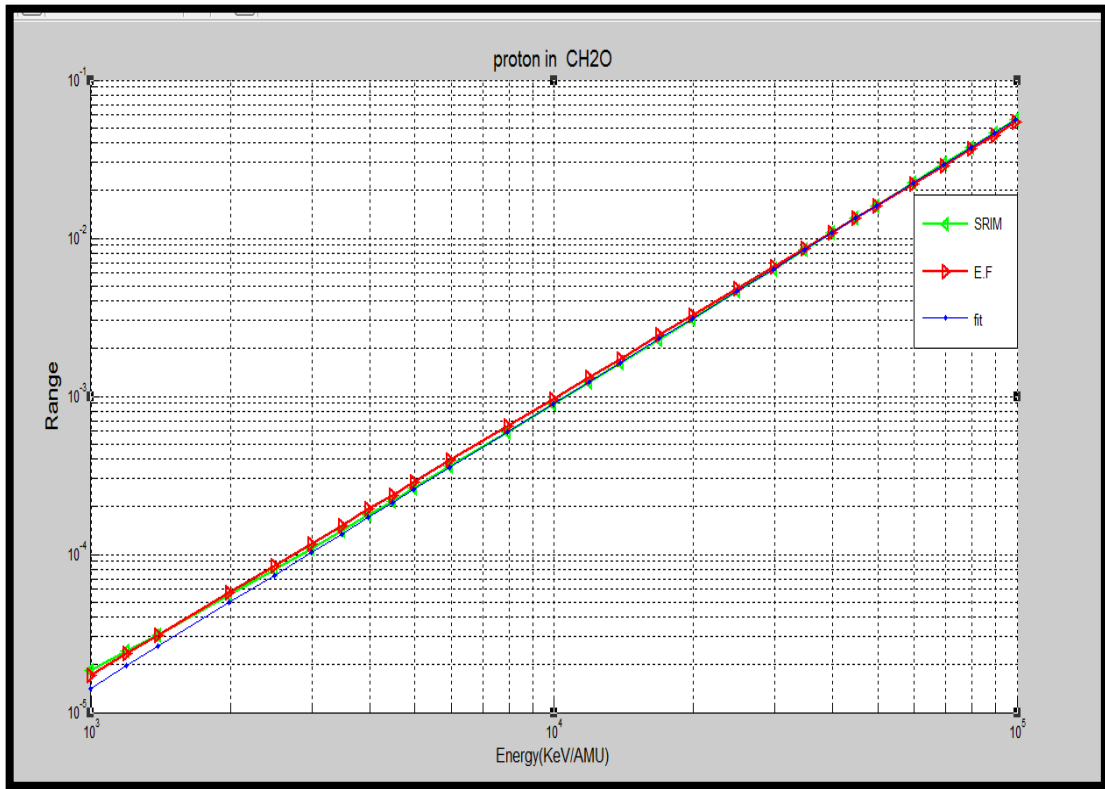
Figure 5 : shows the relationship between the range and energy of compound CH2O was the correlation coefficient (0.999915) and the error ratio(0.000166)
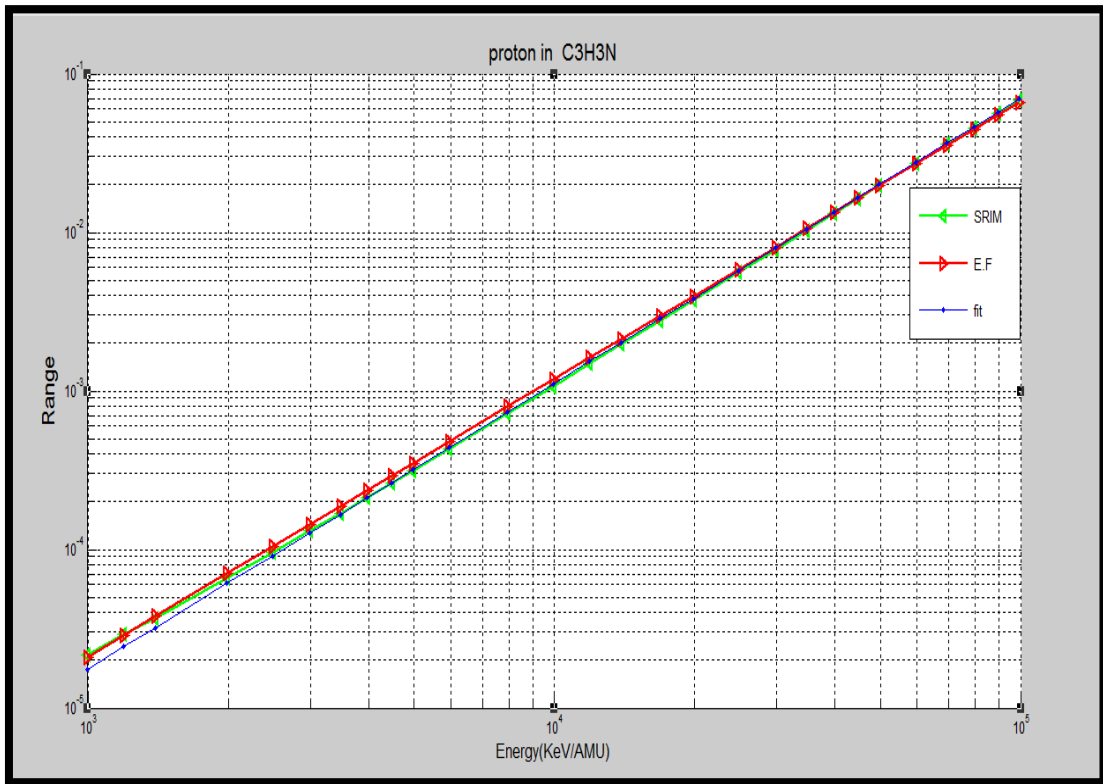
Figure 6 : shows the relationship between the range and energy of compound C3H3N was the correlation coefficient (0.999912) and the error ratio(0.000207)
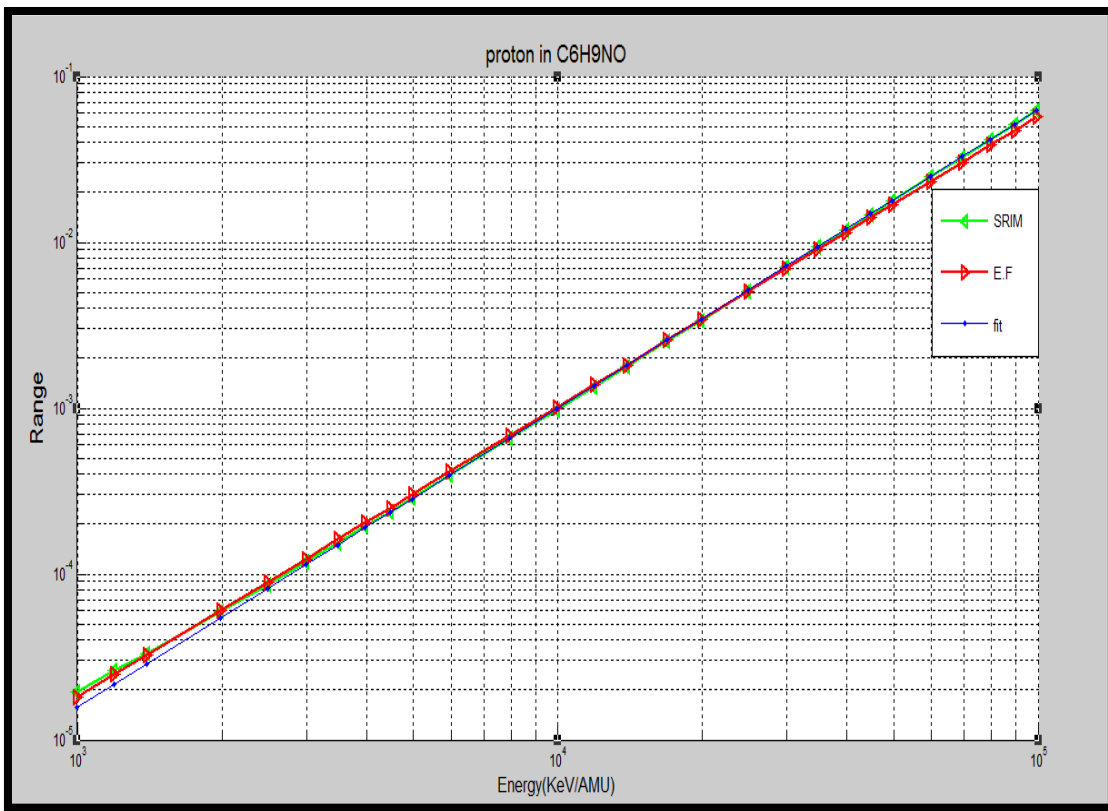
Figure 7 : shows the relationship between the range and energy of compound C6H9NO was the correlation coefficient (0.999909) and the error ratio(0.000191)
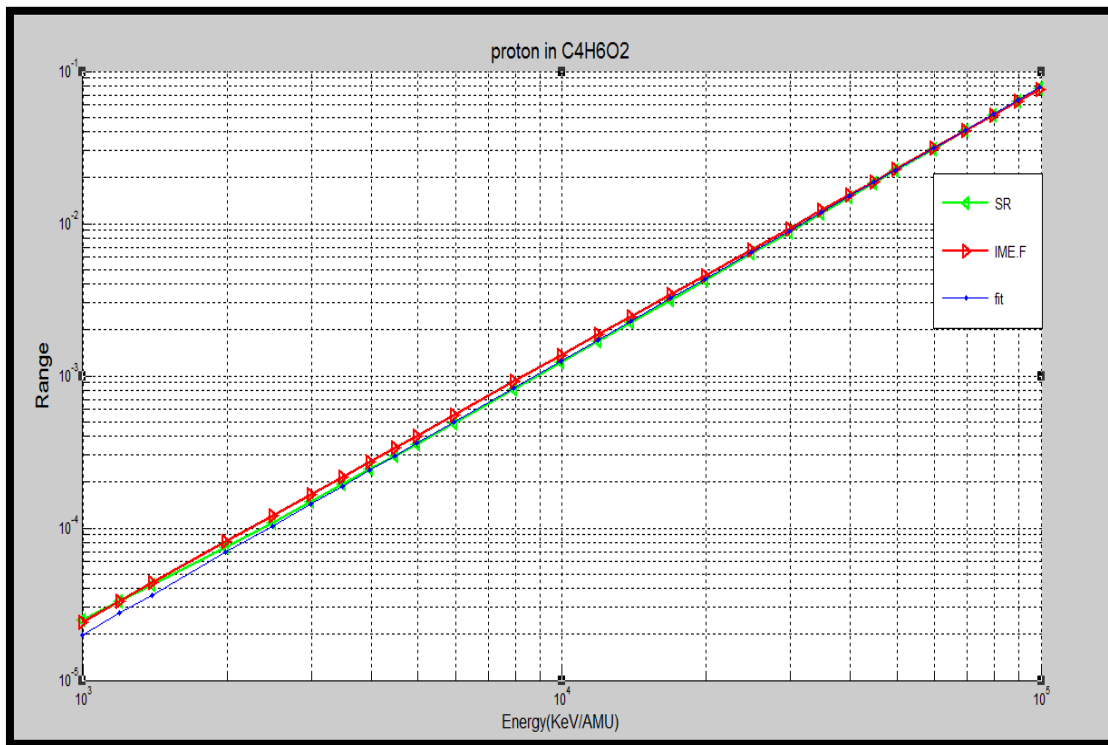
Figure 8 : shows the relationship between the range and energy of compound C4H6O2 was the correlation coefficient (0.999913) and the error ratio(0.000232)
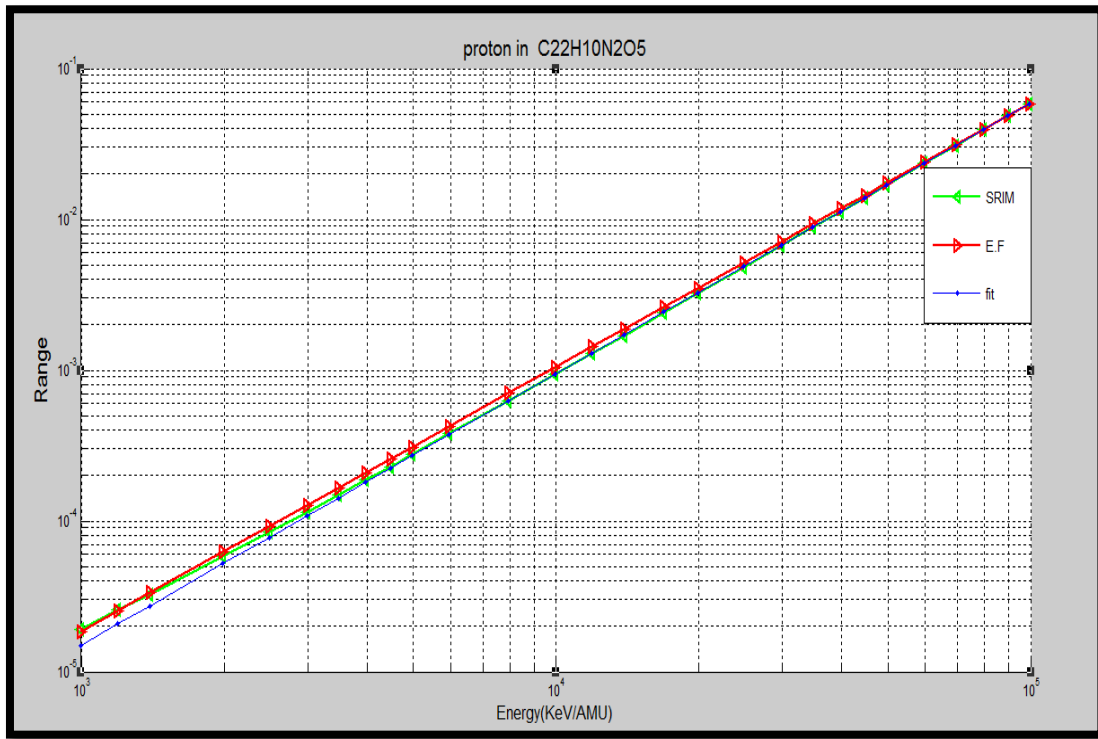
Figure 9 : shows the relationship between the range and energy of compound C22H10N2O5 was the correlation coefficient (0.999919) and the error ratio(0.00017)
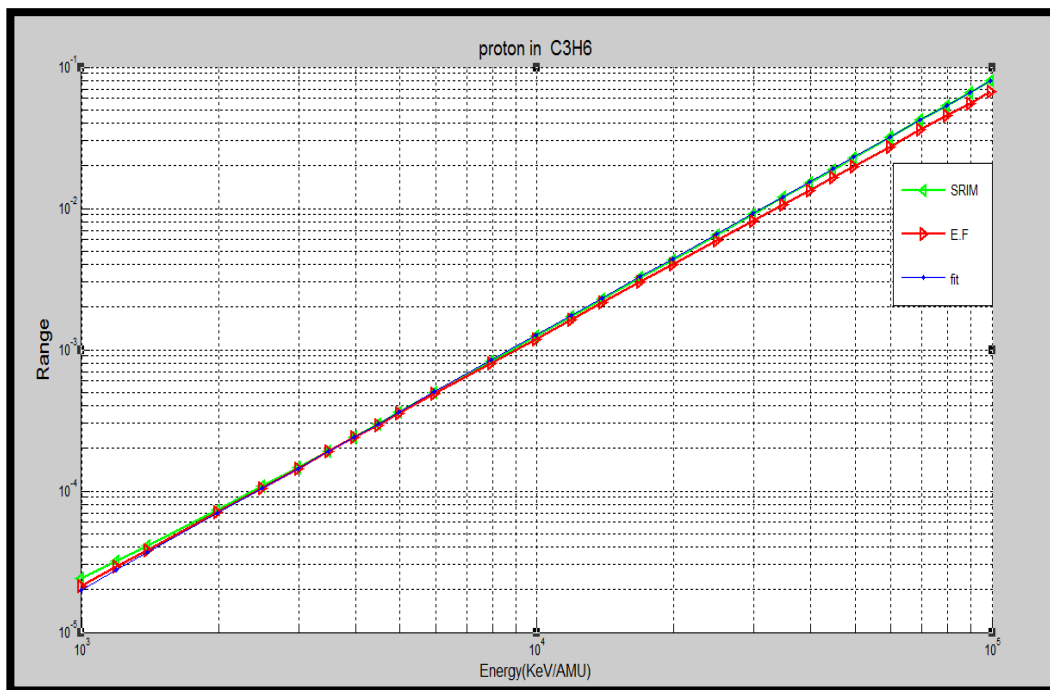

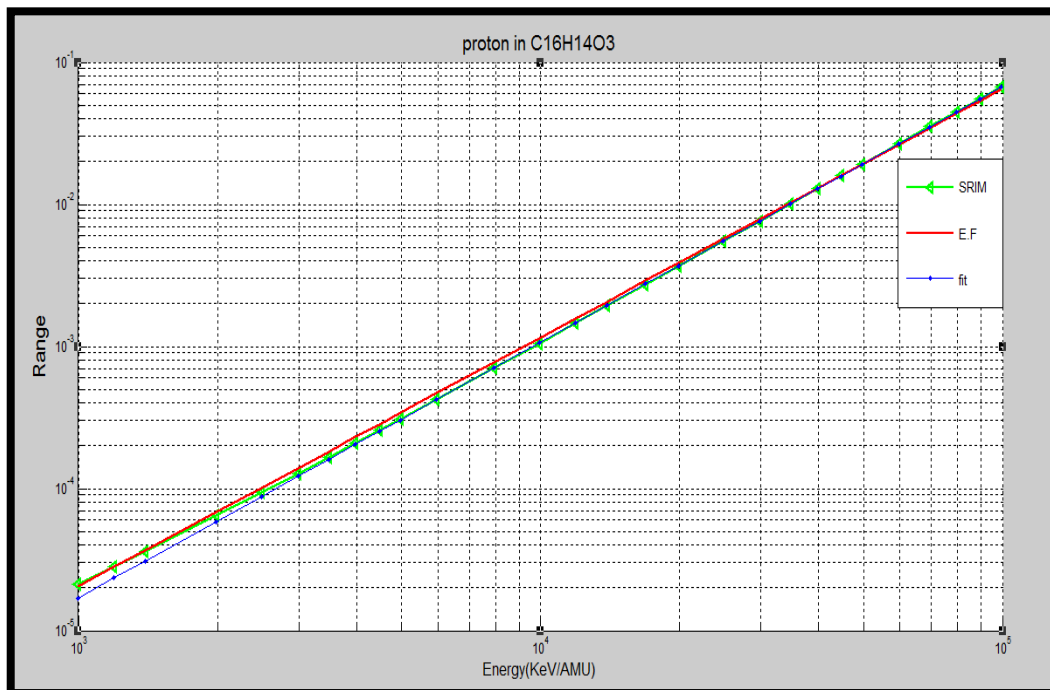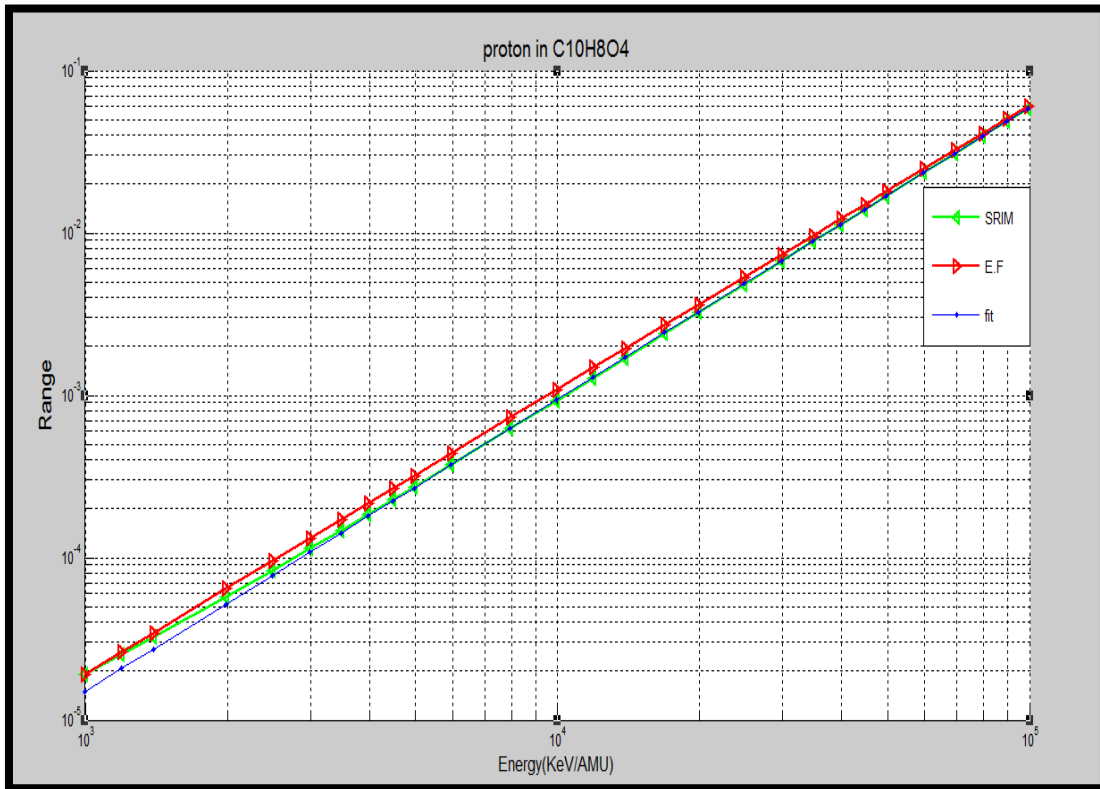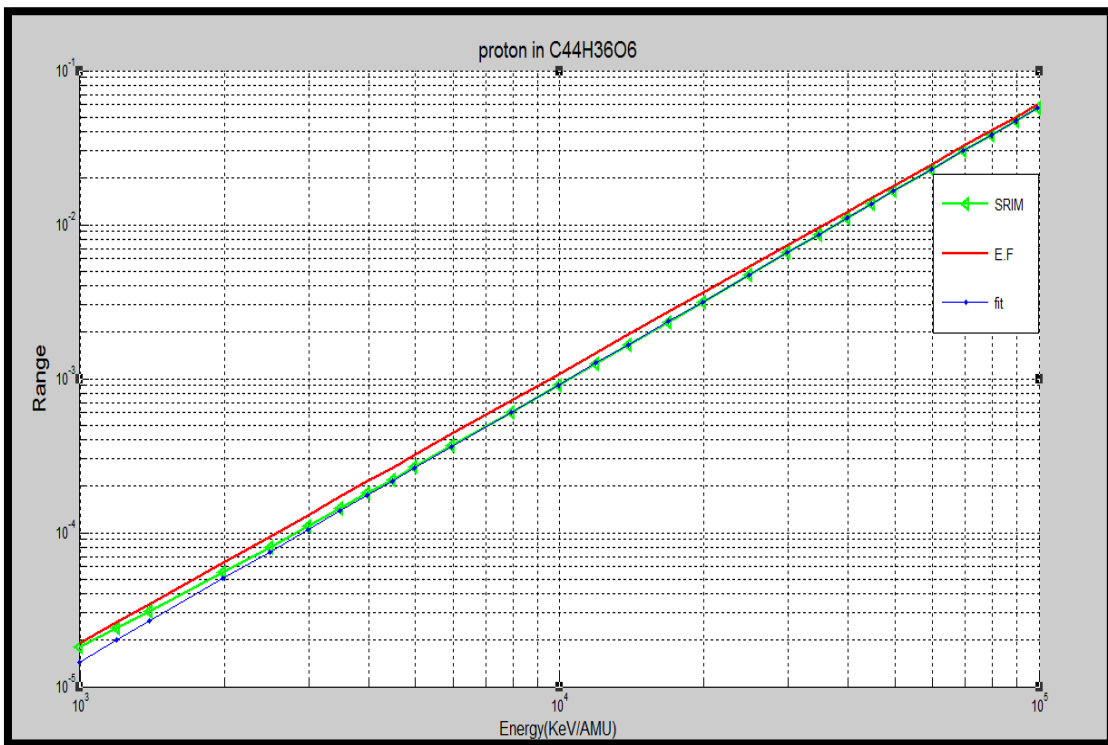*Figure 10 :* shows the relationship between the range and energy of compound C44H36O6 was the correlation coefficient (0.999913) and the error ratio(0.000172)

Table (1)

Energy	function			compound	constants
(1000 - 100000) keV	Power Number 1		$F(x) = ax^b$ or $R(E) = aE^b$	Polypropylene C3H6	RMSE=4.057*10^{-5} a= 7.763*10^{-11} b=1.803
				Polycarbonate C16H14O3	RMSE=3.125*10^{-5} a=9.05*10^{-11} b=1.798
				Mylar C10H8O4	RMSE=2.795*10^{-5} a=6.14*10^{-11} b=1.797
				Polyvinyl alcohol C2H4O	RMSE=2.937*10^{-5} a=6.032*10^{-11} b=1.799
				Polyoxymethylene CH2O	RMSE=2.714*10^{-5} a=5.854*10^{-11} b=1.797

Table (2)

Energy	function			ompound	constants
(1000 - 100000) keV	Power Number 1		$$F(x) = ax^b$$ or $$R(E) = aE^b$$	Polyacrylonitrile C3H3N	RMSE=3.196*10⁻⁵ a= 7.028*10⁻¹¹ b=1.803
				Polyvinylpyrrolidone C6H9NO	RMSE=3.018*10⁻⁵ a=6.32*10⁻¹¹ b=1.8
				Polyvinylacetate C4H6O2	RMSE=3.77*10⁻⁵ a=8.003*10⁻¹¹ b=1.798
				Kapton C22H10N2O5	RMSE=2.788*10⁻⁵ a=6.216*10⁻¹¹ b=1.769
				Bakelite C44H36O6	RMSE=2.64*10⁻⁵ a=5.921*10⁻¹¹ b=1.798

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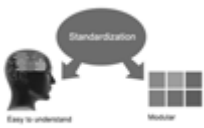
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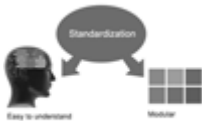
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"
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3. Submission of Manuscripts,

4. Manuscript's Category,

5. Structure and Format of Manuscript,

6. After Acceptance.

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Final Points:

A purpose of organizing a research paper is to let people to interpret your effort selectively. The journal requires the following sections, submitted in the order listed, each section to start on a new page.

The introduction will be compiled from reference matter and will reflect the design processes or outline of basis that direct you to make study. As you will carry out the process of study, the method and process section will be constructed as like that. The result segment will show related statistics in nearly sequential order and will direct the reviewers next to the similar intellectual paths throughout the data that you took to carry out your study. The discussion section will provide understanding of the data and projections as to the implication of the results. The use of good quality references all through the paper will give the effort trustworthiness by representing an alertness of prior workings.

Writing a research paper is not an easy job no matter how trouble-free the actual research or concept. Practice, excellent preparation, and controlled record keeping are the only means to make straightforward the progression.

General style:

Specific editorial column necessities for compliance of a manuscript will always take over from directions in these general guidelines.

To make a paper clear

· Adhere to recommended page limits

Mistakes to evade

- Insertion a title at the foot of a page with the subsequent text on the next page
- Separating a table/chart or figure - impound each figure/table to a single page
- Submitting a manuscript with pages out of sequence

In every sections of your document

· Use standard writing style including articles ("a", "the," etc.)

· Keep on paying attention on the research topic of the paper

· Use paragraphs to split each significant point (excluding for the abstract)

· Align the primary line of each section

· Present your points in sound order

· Use present tense to report well accepted

· Use past tense to describe specific results

· Shun familiar wording, don't address the reviewer directly, and don't use slang, slang language, or superlatives

· Shun use of extra pictures - include only those figures essential to presenting results

Title Page:

Choose a revealing title. It should be short. It should not have non-standard acronyms or abbreviations. It should not exceed two printed lines. It should include the name(s) and address (es) of all authors.

Abstract:

The summary should be two hundred words or less. It should briefly and clearly explain the key findings reported in the manuscript--must have precise statistics. It should not have abnormal acronyms or abbreviations. It should be logical in itself. Shun citing references at this point.

An abstract is a brief distinct paragraph summary of finished work or work in development. In a minute or less a reviewer can be taught the foundation behind the study, common approach to the problem, relevant results, and significant conclusions or new questions.

Write your summary when your paper is completed because how can you write the summary of anything which is not yet written? Wealth of terminology is very essential in abstract. Yet, use comprehensive sentences and do not let go readability for briefness. You can maintain it succinct by phrasing sentences so that they provide more than lone rationale. The author can at this moment go straight to shortening the outcome. Sum up the study, with the subsequent elements in any summary. Try to maintain the initial two items to no more than one ruling each.

- Reason of the study - theory, overall issue, purpose
- Fundamental goal
- To the point depiction of the research
- Consequences, including <u>definite statistics</u> - if the consequences are quantitative in nature, account quantitative data; results of any numerical analysis should be reported
- Significant conclusions or questions that track from the research(es)

Approach:

- Single section, and succinct
- As a outline of job done, it is always written in past tense
- A conceptual should situate on its own, and not submit to any other part of the paper such as a form or table
- Center on shortening results - bound background information to a verdict or two, if completely necessary
- What you account in an conceptual must be regular with what you reported in the manuscript
- Exact spelling, clearness of sentences and phrases, and appropriate reporting of quantities (proper units, important statistics) are just as significant in an abstract as they are anywhere else

Introduction:

The **Introduction** should "introduce" the manuscript. The reviewer should be presented with sufficient background information to be capable to comprehend and calculate the purpose of your study without having to submit to other works. The basis for the study should be offered. Give most important references but shun difficult to make a comprehensive appraisal of the topic. In the introduction, describe the problem visibly. If the problem is not acknowledged in a logical, reasonable way, the reviewer will have no attention in your result. Speak in common terms about techniques used to explain the problem, if needed, but do not present any particulars about the protocols here. Following approach can create a valuable beginning:

- Explain the value (significance) of the study
- Shield the model - why did you employ this particular system or method? What is its compensation? You strength remark on its appropriateness from a abstract point of vision as well as point out sensible reasons for using it.
- Present a justification. Status your particular theory (es) or aim(s), and describe the logic that led you to choose them.
- Very for a short time explain the tentative propose and how it skilled the declared objectives.

Approach:

- Use past tense except for when referring to recognized facts. After all, the manuscript will be submitted after the entire job is done.
- Sort out your thoughts; manufacture one key point with every section. If you make the four points listed above, you will need a least of four paragraphs.

- Present surroundings information only as desirable in order hold up a situation. The reviewer does not desire to read the whole thing you know about a topic.
- Shape the theory/purpose specifically - do not take a broad view.
- As always, give awareness to spelling, simplicity and correctness of sentences and phrases.

Procedures (Methods and Materials):

This part is supposed to be the easiest to carve if you have good skills. A sound written Procedures segment allows a capable scientist to replacement your results. Present precise information about your supplies. The suppliers and clarity of reagents can be helpful bits of information. Present methods in sequential order but linked methodologies can be grouped as a segment. Be concise when relating the protocols. Attempt for the least amount of information that would permit another capable scientist to spare your outcome but be cautious that vital information is integrated. The use of subheadings is suggested and ought to be synchronized with the results section. When a technique is used that has been well described in another object, mention the specific item describing a way but draw the basic principle while stating the situation. The purpose is to text all particular resources and broad procedures, so that another person may use some or all of the methods in one more study or referee the scientific value of your work. It is not to be a step by step report of the whole thing you did, nor is a methods section a set of orders.

Materials:

- Explain materials individually only if the study is so complex that it saves liberty this way.
- Embrace particular materials, and any tools or provisions that are not frequently found in laboratories.
- Do not take in frequently found.
- If use of a definite type of tools.
- Materials may be reported in a part section or else they may be recognized along with your measures.

Methods:

- Report the method (not particulars of each process that engaged the same methodology)
- Describe the method entirely
- To be succinct, present methods under headings dedicated to specific dealings or groups of measures
- Simplify - details how procedures were completed not how they were exclusively performed on a particular day.
- If well known procedures were used, account the procedure by name, possibly with reference, and that's all.

Approach:

- It is embarrassed or not possible to use vigorous voice when documenting methods with no using first person, which would focus the reviewer's interest on the researcher rather than the job. As a result when script up the methods most authors use third person passive voice.
- Use standard style in this and in every other part of the paper - avoid familiar lists, and use full sentences.

What to keep away from

- Resources and methods are not a set of information.
- Skip all descriptive information and surroundings - save it for the argument.
- Leave out information that is immaterial to a third party.

Results:

The principle of a results segment is to present and demonstrate your conclusion. Create this part a entirely objective details of the outcome, and save all understanding for the discussion.

The page length of this segment is set by the sum and types of data to be reported. Carry on to be to the point, by means of statistics and tables, if suitable, to present consequences most efficiently.You must obviously differentiate material that would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matter should not be submitted at all except requested by the instructor.

Content
- Sum up your conclusion in text and demonstrate them, if suitable, with figures and tables.
- In manuscript, explain each of your consequences, point the reader to remarks that are most appropriate.
- Present a background, such as by describing the question that was addressed by creation an exacting study.
- Explain results of control experiments and comprise remarks that are not accessible in a prescribed figure or table, if appropriate.
- Examine your data, then prepare the analyzed (transformed) data in the form of a figure (graph), table, or in manuscript form.

What to stay away from
- Do not discuss or infer your outcome, report surroundings information, or try to explain anything.
- Not at all, take in raw data or intermediate calculations in a research manuscript.

- Do not present the similar data more than once.
- Manuscript should complement any figures or tables, not duplicate the identical information.
- Never confuse figures with tables - there is a difference.

Approach
- As forever, use past tense when you submit to your results, and put the whole thing in a reasonable order.
- Put figures and tables, appropriately numbered, in order at the end of the report
- If you desire, you may place your figures and tables properly within the text of your results part.

Figures and tables
- If you put figures and tables at the end of the details, make certain that they are visibly distinguished from any attach appendix materials, such as raw facts
- Despite of position, each figure must be numbered one after the other and complete with subtitle
- In spite of position, each table must be titled, numbered one after the other and complete with heading
- All figure and table must be adequately complete that it could situate on its own, divide from text

Discussion:

The Discussion is expected the trickiest segment to write and describe. A lot of papers submitted for journal are discarded based on problems with the Discussion. There is no head of state for how long a argument should be. Position your understanding of the outcome visibly to lead the reviewer through your conclusions, and then finish the paper with a summing up of the implication of the study. The purpose here is to offer an understanding of your results and hold up for all of your conclusions, using facts from your research and generally accepted information, if suitable. The implication of result should be visibly described. Infer your data in the conversation in suitable depth. This means that when you clarify an observable fact you must explain mechanisms that may account for the observation. If your results vary from your prospect, make clear why that may have happened. If your results agree, then explain the theory that the proof supported. It is never suitable to just state that the data approved with prospect, and let it drop at that.

- Make a decision if each premise is supported, discarded, or if you cannot make a conclusion with assurance. Do not just dismiss a study or part of a study as "uncertain."
- Research papers are not acknowledged if the work is imperfect. Draw what conclusions you can based upon the results that you have, and take care of the study as a finished work
- You may propose future guidelines, such as how the experiment might be personalized to accomplish a new idea.
- Give details all of your remarks as much as possible, focus on mechanisms.
- Make a decision if the tentative design sufficiently addressed the theory, and whether or not it was correctly restricted.
- Try to present substitute explanations if sensible alternatives be present.
- One research will not counter an overall question, so maintain the large picture in mind, where do you go next? The best studies unlock new avenues of study. What questions remain?
- Recommendations for detailed papers will offer supplementary suggestions.

Approach:

- When you refer to information, differentiate data generated by your own studies from available information
- Submit to work done by specific persons (including you) in past tense.
- Submit to generally acknowledged facts and main beliefs in present tense.

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Topics	Grades		
	A-B	**C-D**	**E-F**
Abstract	Clear and concise with appropriate content, Correct format. 200 words or below	Unclear summary and no specific data, Incorrect form. Above 200 words	No specific data with ambiguous information. Above 250 words
Introduction	Containing all background details with clear goal and appropriate details, flow specification, no grammar and spelling mistake, well organized sentence and paragraph, reference cited	Unclear and confusing data, appropriate format, grammar and spelling errors with unorganized matter	Out of place depth and content, hazy format
Methods and Procedures	Clear and to the point with well arranged paragraph, precision and accuracy of facts and figures, well organized subheads	Difficult to comprehend with embarrassed text, too much explanation but completed	Incorrect and unorganized structure with hazy meaning
Result	Well organized, Clear and specific, Correct units with precision, correct data, well structuring of paragraph, no grammar and spelling mistake	Complete and embarrassed text, difficult to comprehend	Irregular format with wrong facts and figures
Discussion	Well organized, meaningful specification, sound conclusion, logical and concise explanation, highly structured paragraph reference cited	Wordy, unclear conclusion, spurious	Conclusion is not cited, unorganized, difficult to comprehend
References	Complete and correct format, well organized	Beside the point, Incomplete	Wrong format and structuring

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