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of Science Frontier Research: B

Chemistry

Nitrite from Wastewater

Pedagogies - A Review Article

Highlights

Flexible Polyether Foam

Removal of Toxic Nitrate

Discovering Thoughts, Inventing Future

VOLUME 17 ISSUE 2 VERSION 1.0

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Chemical Bonding: Time Economic Innovative Pedagogies - A Review Article

By Arijit Das
Ramthakur College

Abstract- In this article, text based learning approaches have been highlighted by innovative and time economic way to enhance interest of students' who belong to paranoia zone in chemical bonding. In this pedagogical survey, I have tried to hub seven (07) time economic pedagogies by including twenty six (26) new formulae. This review explores the results and gives implications for context based teaching, learning and assessment.

Keywords: *chemical education research, engineering UG level students, chemical bonding, hybridization & geometry, molecular orbital theory, bond order, oxide based acid radical, magnetic properties, spin multiplicity, chemical bonds, alkenes and alkynes.*

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Arijit Das

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I. Introduction

The conventional methods[1-7] for determination of hybridization of simple molecules or ions, bond order of diatomic species having (1-20)e$^-$s using M.O.T., bond-order of oxide based acid radicals, prediction of spin state using spin multiplicity value, evaluation of magnetic behaviour of diatomic species having (1-20)e$^-$s with M.O.T., calculation of number bonds in olefinic hydrocarbons and alkynes are time consuming. Keeping this in mind, in this survey, I have introduced some innovative teaching methodologies[8-18] to make chemistry fascinating and time economic. Here, I have tried to discuss them abruptly with different multiple choice questions.

II. Time Economic Innovative Pedagogies

a) *Predicting the Hybridization of Simple Molecules/ions*

In chemistry, hybridization is the concept of mixing atomic orbitals into newly hybrid orbitals suitable for the pairing of electrons to form chemical bonds in valence bond theory (VBT). Hybrid orbitals are differ in energies, shapes, etc., than the component atomic orbitals. Hybrid orbitals are very useful in the explanation of molecular geometry and atomic bonding properties. Prof. Linus Pauling (1931), first proposed the Hybridization in order to explain the structure of molecules such as methane (CH_4) using atomic orbitals. Here, an innovative time economic methodology proposed for the determination of hybridization state .

i. *Prediction of sp, sp^2, sp^3 Hybridization state*

Hybridization is nothing but the mixing of orbital's in different ratio and the newly mixed orbitals called hybrid orbitals. The mixing pattern is as follows:

s + p (1:1) - sp hybrid orbital;

s + p (1:2) - sp^2 hybrid orbital;

s + p (1:3) - sp^3 hybrid orbital

Formula used for the determination of sp, sp^2 and sp^3 hybridization state:

Power on the Hybridization state of the central atom = (Total no of σ bonds around each central atom -1)

All single (-) bonds are σ bond, in double bond (=) there is one σ and 1π, in triple bond (≡) there is one σ and 2π. In addition to these each lone pair (LP) and Co-ordinate bond can be treated as one σ bond subsequently.

Eg.:

1. *In NH_3:* central atom N is surrounded by three N-H single bonds i.e. three sigma (σ) bonds and one lone pair (LP) i.e. one additional σ bond. So, in NH_3 there is a total of four σ bonds [3 bond pairs (BPs) + 1 lone pair (LP)] around central atom N. Therefore, in this case power of the hybridization state of N = 4-1 = 3 i.e. hybridization state = sp^3.
2. *In H_2O:* central atom O is surrounded by two O-H single bonds i.e. two sigma (σ) bonds and two lone pairs i.e. two additional σ bonds. So, altogether in H_2O there are four σ bonds (2 bond pairs + 2 lone pairs) around central atom O, So, in this case power of the hybridization state of O = 4-1 =3 i.e. hybridization state of O in H_2O = sp^3.
3. *In H_3BO_3:* B has 3σ bonds (3BPs but no LPs) and oxygen has 4σ bonds (2BPs & 2LPs) so, in this case power of the hybridization state of B = 3-1 = 2 i.e. B is sp^2 hybridized in H_3BO_3. On the other hand, power of the hybridization state of O = 4-1= 3 i.e. hybridization state of O in H_3BO_3 is sp^3.

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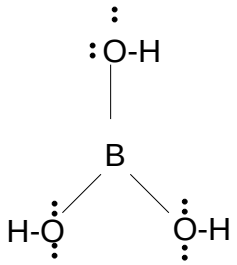
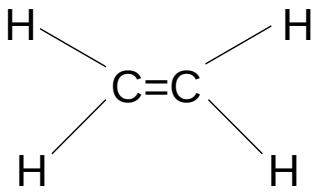


4. *In I-Cl:* I and Cl both have 4σ bonds and 3LPs, so, in this case power of the hybridization state of both I and Cl = 4 - 1 = 3 i.e. hybridization state of I and Cl both are sp^3.

5. *In CH_2=CH_2:* each carbon is attached with 2 C-H single bonds (2 σ bonds) and one C=C bond (1σ bond), so, altogether there are 3 sigma bonds. So, in this case, power of the hybridization state of both C = 3-1 = 2 i.e. hybridization state of both C's are sp^2.



b) Prediction of sp^3d, sp^3d^2, sp^3d^3 Hybridization state

In case of sp^3d, sp^3d^2 and sp^3d^3 hybridization state there is a common term sp^3 for which 4 sigma bonds are responsible. So, in addition to 4 sigma bonds, for each additional sigma, added one d orbital gradually as follows:-

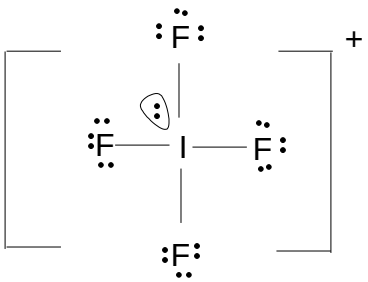
5σ bonds = 4σ bonds + 1 additional σ bond = sp^3d hybridization

6σ bonds = 4σ bonds + 2 additional σ bonds = sp^3d^2 hybridization

7σ bonds = 4σ bonds + 3 additional σ bonds = sp^3d^3 hybridization

Eg:-

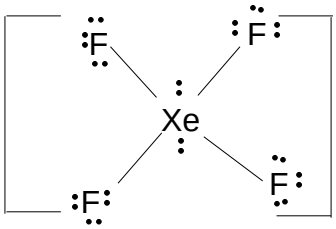
1. *IF_4^+:* I has 7 e^-s in its outermost shell, so, in this case, subtract one e^- from 7 i.e. 7 – 1 = 6. So, out of 6 electrons, 4 electrons form 4 I-F bonds i.e. 4 sigma bonds and there is one LP. So, altogether there are 5 σ bonds. So, 5σ bonds = 4 σ bonds + 1 additional σ bond = sp^3d hybridization".



2. *IF_7:* 7 I-F single bonds i.e. 7σ bonds = 4σ bonds + 3 additional σ bonds = sp^3d^3 hybridization.

3. *ICl_2^-:* I has 7 e^-s in its outermost shell, so, in this case, add one e^- with 7(overall charge on the compound) i.e. 07+1= 08. So, out of 08 electrons, 02 electrons form 02 I-Cl bonds i.e. 02 sigma bonds and there is 03 LPs. So, altogether there are 05σ bonds. So, 5σ bonds = 04 σ bonds + 01 additional σ bond = sp^3d hybridization.

4. *XeF_4:* Xe, an inert gas, consider 8 e^-s in its outermost shell, 04 of which form 04 Xe-F sigma bonds and there is two LPs, i.e. altogether there is 06 σ bonds = 04 σ bonds + 02 additional σ bonds = sp^3d^2 hybridization.



In case of determination of the hybridization state by using the above method, one must have a clear idea about the outermost electrons of different family members in the periodic table as follows:

Family	Outermost electrons
Carbon family	04
Nitrogen family	05
Oxygen family	06
Halogen family	07
Inert gas family	08

In case of cationic species, requisite electron/electrons must be removed from the outermost orbit of the central atom and incase of anionic species, added requisite electron with the outermost electrons of the central atom. Examples have been explored in Table-1.

Table 1: (σ bonds and corresponding hybridization State)

Total number of sigma (σ) bonds	Nature of Hybridization State	Examples
2	sp	$BeCl_2$, $HgCl_2$, C_2H_2, CO_2, CO, $CdCl_2$, $ZnCl_2$ etc.
3	sp^2	BCl_3, $AlCl_3$,C_2H_4,C_6H_6,SO_2,SO_3,HNO_3, H_2CO_3,$SnCl_2$, $PbCl_2$ etc.
4	sp^3	NH_4^+, BF_4^-, H_2S, H_2SO_4, $HClO_4$, PCl_3, NCl_3, $AsCl_3$, $HClO_3$, ICl_2^+,OF_2,$HClO_2$, SCl_2, HClO, ICl, XeO_3 etc.
5	sp^3d	PCl_5, $SbCl_5$, SF_4, ClF_3, BrF_3, XeF_2, ICl_2^- etc.
6	sp^3d^2	SF_6, AlF_6^{3-}, SiF_6^{2-}, PF_6^-, IF_5, BrF_5, $XeOF_4$, XeF_4, BrF_4^-, ICl_4^- etc.
7	sp^3d^3	IF_7, XeF_6 etc.

Geometry of simple molecules or ions:

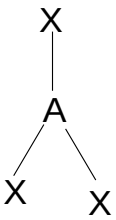
In absence of lone pair of electrons a molecule or ion exhibit regular geometry. For sp, sp^2, sp^3, sp^3d, sp^3d^2 and sp^3d^3 hybridization state, geometry will be linear, trigonal planar, tetrahedral, trigonal bipyramid, octahedral and pentagonal bipyramid respectively, where as for the same hybridization state in presence of lone pair of electrons they exhibit sub normal geometry (Fig-1, Table-2).

Table 2: Hybridization, Molecular Geometry and Bond Angles without/with lone pair of electrons

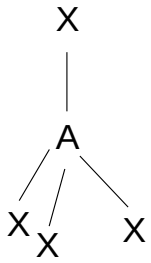
Hybridization	LP	Molecular Geometry (Regular/Normal)	Approximate Bond Angles (Degree)	Examples	LP	Molecular Geometry (Sub-normal)	Approximate Bond Angles (Degree)	Example
sp	0	Linear	180	CO_2, CS_2, $BeCl_2$, $HgCl_2$	-	-	-	-
sp^2	0	Trigonal Planar or Triangular planar	120	BH_3, $AlCl_3$, C_2H_4, BCl_3, BF_3, NO_3^-, CO_3^{2-}	01	Angular or V-shape	<120	SO_2, NO_2^-
sp^3	0	Tetrahedral	109.5	BH_4^-, BF_4^-, $SnCl_4$, H_2SO_4 $HClO_4$, $SiCl_4$	01	Pyramidal	<109.5	NH_3, PH_3, AsH_3
					02	Bent shape or V-shape	<109.5	H_2O, H_2S, H_2Se
					03	Linear	180	ICl,BrF, ClF
sp^3d	0	Trigonal bipyramid	120 (equatorial) 90 (axial)	PF_5, PCl_5	01	See-Saw	<120(equatorial) <90 (axial)	SF_4
					02	T-shape	<90	ICl_3,F_3Cl
					03	Linear	180	XeF_2,I_3^-
sp^3d^2	0	Octahedral	90	SF_6, WF_6, SeF_6, $SnCl_6^{2-}$	01	Square pyramidal	<90	IF_5,BrF_5
					02	Square planar	90	XeF_4
sp^3d^3	0	Pentagonal bipyramid	72 & 90	IF_7	01	Pentagonal Pyramidal or Distorted octahedral	72 & 90	XeF_6

Regular/Normal Molecular Geometry without Lone pair of electrons:

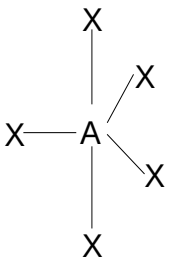
X-A-X
(Linear, sp, LP=0)



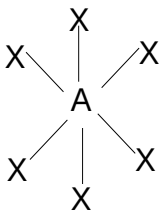
(Trigonal planar, sp^2 , LP=0)



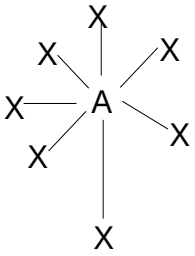
(Tetrahedral, sp^3, LP=0)



(Trigonal bipyramidal, sp^3d, LP=0)

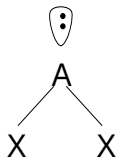


(Octahedral, sp^3d^2, LP=0)

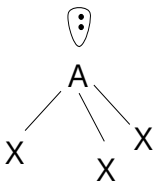


(Petntagonal bipyramidal,sp^3d^3,LP =0)

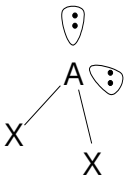
Sub-normal Molecular Geometry with Lone pair of electrons:



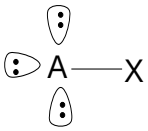
(Bent or V shape, sp^2, LP = 01)



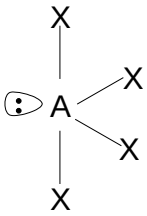
(Pyramidal, sp^3, LP=01)



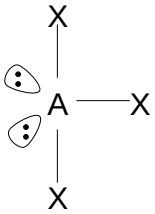
(Bent or V shape, sp^3, LP=02)



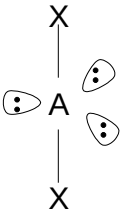
(Linear,sp^3,LP=03)



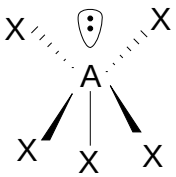
(See Saw, sp^3d, LP=01)



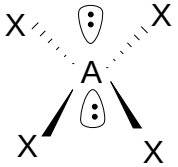
(T shape, sp^3d, LP=02)



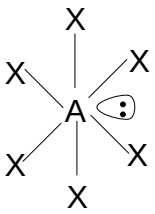
(Linear,sp^3d,LP=03)



(Square Pyramidal, sp^3d^2, LP=01)



(Square planar, sp^3d^2, LP=02)



(Pentagonal Pyramidal, sp^3d^3, LP=01)

Fig. 1: Pictorial diagram of molecular geometry

Problems on Hybridization and Geometry:

Q.1. In allene, hybridization of central and terminal carbons, respectively, are
a. sp and sp^2 b. sp^2 and sp^2 c. sp and sp^3 d. sp^2 and sp^3

Ans: a. sp and sp^2 (Allene $H_2C{=}C{=}CH_2$)
sp^2 sp sp^2

Q.2. The species which has a square planar structure is
a. SF_4 b. BF_4^- c. XeF_2 d. XeF_4
Ans: d. XeF_4 (Hybridization sp^3d^2, LP = 02, square planar geometry)

Q.3. The hybrid bond orbitals used by chlorine in forming ClF_3 are of the type
a. sp^3 b. sp^2 c. sp^3d d. sp^3d^2
Ans: c. sp^3d (In ClF_3 - 5σ bonds around Cl atom.
So, 5σ bonds = 4 σ bonds + 1 additional σ bond = sp^3d hybridization)

Q.4. Which are the species in which sulphur undergoes sp^3 hybridization ?
A. SF_4 B. SCl_2 C. SO_4^{2-} D. H_2S
a. A and C b. B, C and D c. A, B and D d. C and D
Ans: b. B, C and D (SF_4 - 5σ bonds around S atom sp^3d hybridization)

Q.5. Which of the following compounds show linear geometry ?
a. BeH_2 b. CH_4 c. XeF_2 d. H_2O
Ans: a. & c. (BeH_2 – hybridization sp, LP = 0, regular shape - Linear ; XeF_2 - hybridization sp^3d, LP = 03, sub-normal shape – Linear)

Q.6.Which of the following compound will show square pyramidal structure ?
a. XeF_4 b. IF_5 c. IF_7 d. XeF_6
Ans: b. IF_5 (6σ bonds around I atom sp^3d^2 hybridization, LP = 01, square pyramidal geometry)

III. Predicting the Bond-Order of Diatomic Species without Molecular Orbital Theory(MOT)

Bond-order usually predicted from the Molecular Orbital Theory. Molecular Orbital Theory (M.O.T.) was first proposed by Friedrich Hund and Robert Mulliken in 1933. They developed an approach to covalent bond formation which is based upon the effects of the various electron fields upon each other and which employs molecular orbital rather than atomic orbital. Each such orbital characterizing the molecule as a whole is described by a definite combination of quantum numbers and possesses relative energy value.

a) For diatomic species having (1-20)e⁻s

Graphical Representation of B.O. with number of electrons

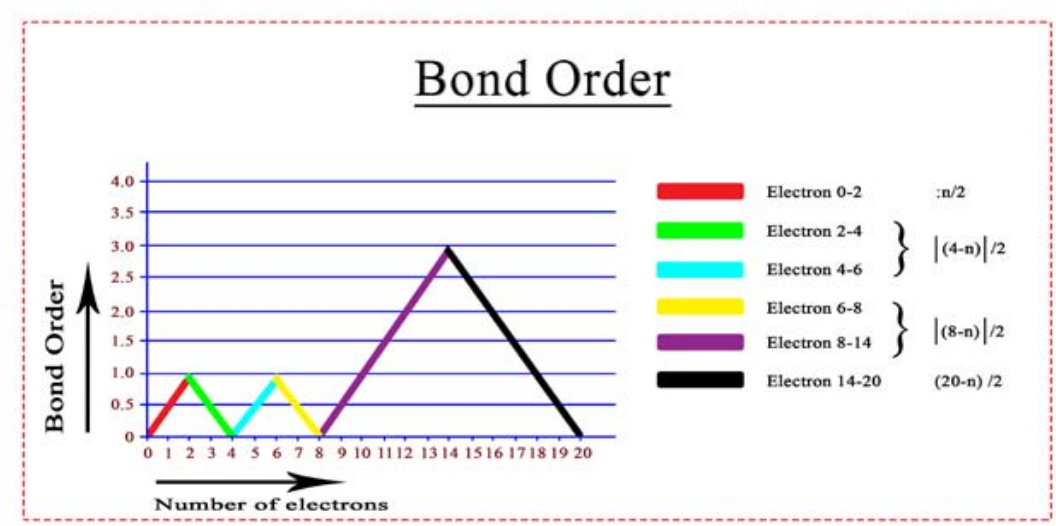


Fig. 2: (B.O. vs number of electrons)

The graphical representation presented in Fig.2 shows that bond-order gradually increases to 1 in the range (0-2) electrons then falls to zero in the range (2-4) electrons then it further rises to 1 for (4-6) electrons and once again falls to zero for (6-8) electrons then again rises to 3 in the range (8-14) electrons and then finally falls to zero for (14-20) electrons. For total no of electrons 2, 6 and 14, one can use multiple formulae, because they fall in the overlapping region in which they intersect with each other.

First of all I classify the molecules or ions into the following four (4) types based on total number of electrons present in them.

i) *Molecules and ions having total no of electrons within the range (1-2)*
In such case *Bond order = n/2;* [Where n = Total no of electrons]
Eg: H_2 (Total e⁻s = 2), Therefore B.O. = n/2 = 2/2 = 1

ii) *Molecules and ions having total no of electrons within the range (2-6)*
In such case *Bond order = I 4- n I / 2;*
[Where n = Total no of electrons, 'I I' indicates Mod function i.e. the value of bond order is always positive]
Eg: Li_2^+(5e⁻s) Therefore B.O. = I 4-5 I / 2 = 1/2 = 0.5.

iii) *Molecules and ions having total no of electrons within the range (6-14)*
In such case *Bond order = I 8-n I / 2*
Eg: CO (Total e⁻s = 6+8=14), Therefore B.O.= I 8-14 I / 2 = 3

iv) *Molecules and ions having total no of electrons within the range (14-20)*
In such case *Bond order = (20-n) / 2*; [Where n = Total no of electrons]
Eg: NO (Total e⁻s = 15), Therefore B.O. = 20-15/2 = 2.5

If bond order is zero, the molecule is unstable (does not exist), whereas, a positive value of bond order reveals that the molecule exists and is stable (Table-3).

b) Problems on bond order of diatomic species
Q.1. The bond order of N_2, O_2, N_2^-, O_2^- varies as
a. $N_2 > N_2^- > O_2 > O_2^-$ b. $O_2 > N_2 > O_2^- > N_2^-$ c. $N_2 > O_2 > N_2^- > O_2^-$ d. $N_2^- > N_2 > O_2^- > O_2$
Ans: a. $N_2 > N_2^- > O_2 > O_2^-$
B.O. – 3.0 2.5 2.0 1.5

Q.2. Among the following species, the order of first ionization energy (IE_1) is
a. $O_2 < O_2^+ < O_2^-$ b. $O_2^+ < O_2^- < O_2$ c. $O_2^- < O_2 < O_2^+$ d. $O_2 < O_2^- < O_2^+$
Ans: c. $O_2^- < O_2 < O_2^+$ - IE_1 (Bond order α IE_1 ; Bond order trend is 1.5<2.0<2.5)

Q.3. Which of the following is the correct order of their stability ?

a. $CN < NO^+ < NO^-$ b. $NO^- < CN < NO^+$ c. $NO^+ < CN < NO^-$ d. $CN < NO^- < NO^+$

Ans: b. $NO^- < CN < NO^+$ - stability (Bond order α stability ; Bond order trend is 2.0<2.5<3.0)

Q.4. In which case bond order increases ?

a. O_2 changes to O_2^+ b. N_2 changes to N_2^+ c. NO changes to NO^- d. In all cases

Ans: a. O_2 changes to O_2^+ (bond order increases from 2.0 to 2.5)

Q.5. Which of the following is the correct order of their stability ?

a. $N_2 > N_2^+ > N_2^-$ b. $N_2 > N_2^- > N_2^+$ c. $N_2^+ > N_2 > N_2^-$ d. None of these

Ans: a. $N_2 > N_2^+ > N_2^-$ (Bond order of N_2 = 3.0, N_2^+ & N_2^- = 2.5; Bond order α stability; but when bond order be same then cationic species will have higher stability than anionic species due to increase in electron in higher energetic ABMO in anionic species)

Table 3: [Bond order values of diatomic species having (1-20)e⁻s]

Species (Molecules or ions)	Total Number of e⁻s (n)	Bond-Order (B.O.)
Bond-Order Values for the species having (1-2)e⁻s ; Bond order = n/2		
H_2^+	1	0.5
H_2, He_2^{2+}	2	1
Bond-Order Values for the species having (2-6)e⁻s ; Bond order = | 4- n | / 2		
H_2^-,He_2^+	3	0.5
He_2,	4	0
Li_2^+,He_2^-	5	0.5
Li_2, He_2^{2-}, Be_2^{2+}	6	1
Bond-Order Values for the species having (6-14)e⁻s ; Bond order = | 8- n | / 2		
Be_2^+, Li_2^-	7	0.5
Be_2, Li_2^{2-}	8	0
Be_2^-, B_2^+	9	0.5
B_2, Be_2^{2-}, HF	10	1
B_2^-, C_2^+	11	1.5
C_2, B_2^{2-}, N_2^{2+}, CN^+	12	2
C_2^-, N_2^+	13	2.5
N_2, CO, NO^+, C_2^{2-}, CN^-,O_2^{2+}	14	3
Bond-Order Values for the species having (14-20)e⁻s ; Bond order = (20-n) / 2		
N_2^-, NO, O_2^+	15	2.5
NO^-, O_2	16	2
O_2^-	17	1.5
F_2, O_2^{2-}, HCl	18	1
F_2^-	19	0.5
Ne_2	20	0

III. Predicting Bond-Order of Oxide based Acid Radicals

In case of oxide based acid radicals

Bond Order (B.O.) = Valency of the peripheral atom + (Charge on Acid Radical / Total number of peripheral atoms)

Eg:

ClO_4^-: (Valency of one Peripheral atom Oxygen = 2, Charge on acid radical = -1, Total Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-1/4) = 1.75

ClO_3^-: (Valency of one Peripheral atom Oxygen = 2, Charge on acid radical = -1, Total Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-1/3) = 1.66

ClO_2^-: (Valency of one Peripheral atom Oxygen = 2, Charge on acid radical = -1, Total Number of Peripheral atoms = 02), Therefore B.O. = 2 + (-1/2) = 1.5

AsO_4^{3-}: (Valency of one Peripheral atom Oxygen = 2, Charge on acid radical = -3, Total Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-3/4) = 1.25

AsO_3^{3-}: (Valency of one Peripheral atom Oxygen = 2, Charge on acid radical = -3, Total Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-3/3) = 1.0

SO_4^{2-}: (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = -2, Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-2/4) = 1.5

SO_3^{2-}: (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = -2, Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-2/3) = 1.33

PO_4^{3-}; (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = -3, Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-3/4) = 1.25

BO_3^{3-}; (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = -3, Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-3/3) = 1

CO_3^{2-}; (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = -2, Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-2/3) = 1.33

SiO_4^{4-}: (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = - 4, Number of Peripheral atoms = 04), Therefore B.O. = 2 + (- 4/4) = 1

Bond order is a measure of the strength of the bond between two atoms. Bond order can be applicable to make a comparison of some characteristics between (among) the molecules as

B.O. α 1 / Bond length (BL) or Bond distance (BD);
B.O. α Bond strength (BS);
B.O. α Bond dissociation Energy (BDE);
B.O. α Bond Energy (BE);
B.O. α Ionization Energy (IE);
B.O. α Thermal Stability;
B.O. α 1 / Reactivity (R)

Correlation among / between Literature values of bond-distances of some oxide based acid radicals with their predicted bond order values:

Literature values of the Cl-O average bond lengths in ClO_4^-,ClO_3^- and ClO_2^-; As-O bond lengths in AsO_4^{3-} and AsO_3^{3-} with respect to their bond order values suggest that with increasing bond-order M-O bond length (Where M = Cl, As etc.) decreases which is shown in Table-4.

Table 4: (Correlation of some bond-distances with their predicted bond order values)

Oxide Based Acid Radicals	Bond-Order Values	Avg. M-O Bond-Distances As per Literature (Å)	Remarks
ClO_4^-	1.75	1.50	Increasing Bond-Order decreases Bond Length
ClO_3^-	1.6	1.57	
ClO_2^-	1.5	1.64	
AsO_4^{3-}	1.25	1.75	
AsO_3^{3-}	1.0	1.77	

Correlation among / between Literature values of bond dissociation energy (KJ mol^{-1}) of some molecules or ions with their predicted bond order values (Table-5):

Table 5: (Correlation of some bond dissociation energy with their predicted bond order values)

Molecules or ions	Bond-Order Values	Dissociation energy (KJ mol^{-1})	Remarks
O_2^+	2.5	642.9	Increasing Bond-Order increases Bond dissociation energy (BDE)
O_2	2.0	493.6	
O_2^-	1.5	395.0	
NO^+	3.0	1046.9	
NO	2.5	826.9	
NO^-	2.0	487.8	

IV. Magnetic Behavior of Diatomic Species without Molecular Orbital Theory(MOT)

The present study involves three new formulae by just manipulating the number of unpaired electrons (n) using mod function (based on Applied Mathematics) and by means of these n values one can easily stumble the magnetic moment values in Bohr-Magneton using spin only formula $\mu_s = \sqrt{n(n+2)}$ B.M., where B.M. = Bohr Magneton = Unit of Magnetic Moment, n = number of unpaired electrons.

First of all we classify the molecules or ions depending on the total number of electrons present in them in the following three (03) sets.

Set-1: Molecules or ions having (1-3)e^-s, (3-5)e^-s, (5-7)e^-s, (7-10)e^-s, (13-16)e^-s

Set-2: Molecules or ions having (10-13)e^-s and (16-19)e^-s

Set-3: Molecules or ions having 20 e^-s

Then for different set we have to use three different formulae to calculate the number of unpaired electrons which have been presented in Table-6 and thus magnetic moment (μ_s in B.M.) can be evaluated in the following way:

a) *F-1(For Set-1) - for the determination of number of unpaired electrons (n) of molecules or ions having total number of electrons (1-3), (3-5), (5-7), (7-10) and (13-16)e^-s*

In this case, the number of unpaired electrons n = [I (ND - total e^-s) I]

Here, ND = next digit i.e. digit next to minimum digit and 'I I' indicates mod function.

Eg: Molecules or ions having (1-3)e^-s, in this case ND = 2 because here minimum digit is 1.

Eg. He_2^+ (3e^-s), the total number of electrons will be 3, ND = 2, Hence, unpaired electron n = I (ND - total e^-s) I = I (2-3) I = 1. Hence, Magnetic Moment $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{}$ 1(1+2) BM = $\sqrt{3}$ BM = 1.73BM.

For the molecules or ions containing (3-5)e^-s, (5-7)e^-s, (7-10)e^-s, and (13-16)e^-s the ND value will be 4, 6, 8 and 14 respectively.

Hence, the value of n = [I (4-total e^-s) I]; [I(6- total e^-s)I] [I(8-total e^-s)I] and [I(14- total e^-s)I] respectively.

b) *F-2(For Set-2) - for the determination of number of unpaired electrons (n) of molecules or ions having total number of electrons (10-13) and (16-19)*

In this case, the number of unpaired electrons n = [I (PD - total e^-s) I]

Here, PD = Penultimate electron digit (i.e. before last electron).

Eg: for C_2^- (13e^-s), the total number of electrons will be 13, PD = 12

Hence, unpaired electron n = I (12 - total e^-s) I = I (12-13) I = 1

Hence, Magnetic Moment $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{}$ 1(1+2) BM = $\sqrt{3}$ BM = 1.73BM

For F_2 (18e^-s), the total number of electrons will be 18, PD = 18

Hence, unpaired electron n = I (18 - total e^-s) I = I (18-18) I = 0

Hence, Magnetic Moment $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{}$ 0(0+2) BM = 0 BM = Diamagnetic in nature.

c) *F-3(For Set-3) - for the determination of number of unpaired electrons (n) of molecules or ions having total number of electrons 20*

In this case, the number of unpaired electrons n = [(20 - total e^-s)]

Eg: for Ne_2 (20e^-s), the total number of electrons will be 20,

Hence, unpaired electron n = (20 - total e^-s) = (20-20) = 0

Hence, Magnetic Moment $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{}$ 0(0+2) BM = 0 BM = Diamagnetic in nature.

Table 6: (Magnetic moments of diatomic species)

Species (Molecules or ions)	Total Number of e⁻s	Number of unpaired electrons (n)	Magnetic moment (μ_s) in Bohr Magneton (B.M.)	Remark on magnetic behavior
H_2^+	1	1	1.73	Para magnetic
H_2, He_2^{2+}	2	0	0	Diamagnetic
H_2^-, He_2^+	3	1	1.73	Para magnetic
He_2,	4	0	0	Diamagnetic
Li_2^+,He_2^-	5	1	1.73	Para magnetic
Li_2, He_2^{2-}, Be_2^{2+}	6	0	0	Diamagnetic
Be_2^+,Li_2^-	7	1	1.73	Para magnetic
Be_2,Li_2^{2-}	8	0	0	Diamagnetic
Be_2^-,B_2^+	9	1	1.73	Para magnetic
B_2, Be_2^{2-}, HF	10	2	2.82	Para magnetic
B_2^-,C_2^+	11	1	1.73	Para magnetic
C_2,B_2^{2-},N_2^{2+}, CN^+	12	0	0	Diamagnetic
C_2^-,N_2^+	13	1	1.73	Para magnetic
N_2,CO,NO^+,C_2^{2-},CN^-,O_2^{2+}	14	0	0	Diamagnetic
N_2^-,NO,O_2^+	15	1	1.73	Para magnetic
NO^-,O_2	16	2	2.82	Para magnetic
O_2^-	17	1	1.73	Para magnetic
F_2,O_2^{2-},HCl	18	0	0	Diamagnetic
F_2^-	19	1	1.73	Para magnetic
Ne_2	20	0	0	Diamagnetic

Problems on Magnetic behavior of diatomic species:

Q.1. Which of the following species is diamagnetic ?

a. B_2 b. N_2^+ c. N_2^- d. N_2^{2+}

Ans: d. N_2^{2+} (Total electrons 12, n = 0, Magnetic moment, μ_s = 0 B.M.)

Q.2. Number of unpaired electrons in CO molecule is

a. 0 b.1 c. 2 d. 3

Ans: a. 0 (Table - 6)

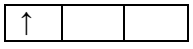
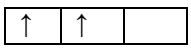
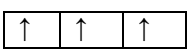
V. Evaluating Spin Multiplicity

Spin-multiplicity value and its corresponding spin state was first discovered by Friedrich Hund in 1925. The formula which is generally used for the prediction of spin multiplicity value is [(2S+1), where S = Σs = total spin quantum no] is time consuming. To keep the matter in mind a simple innovative method has to be introduced for calculation of spin-multiplicity value and thus its corresponding spin state, shown in Table-7, in the easiest way by ignoring the calculation of total spin quantum number (S = Σs).

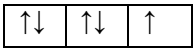
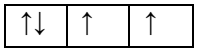
First of all we should classify the species (atoms, molecules, ions or complexes) for which spin multiplicity value should be evaluated into three types based on the nature of alignment of unpaired electrons present in them.

a) Species having unpaired electrons in upward alignment (↑)

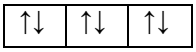
In this case, spin multiplicity = (n+1); where n = number of unpaired electrons

Spin multiplicity = (n +1) = (1+1) = 2 (spin state = doublet); (2+1) = 3 (spin state = triplet) and (3 + 1) = 4 (spin state = quartet) respectively.

Spin multiplicity = (n +1) = (2 + 1) = 3 (in this case ignore paired electrons) (spin state = triplet) and (1+1) = 2 (spin state = doublet)

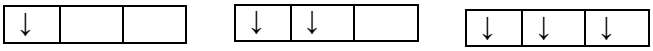


Spin multiplicity = (n +1) = (0 + 1) = 1 (spin state = singlet)

b) Species having unpaired electrons in downward alignment (↓)

In this case spin multiplicity = (-n+1)

Here (-ve) sign indicate downward arrow.



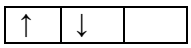
Spin multiplicity = (-n +1) = (-1 + 1) = 0; (-2 + 1) = -1 and (-3 + 1) = -2 respectively.

Spin multiplicity = (-n + 1) = (-2 + 1) = -1(ignore paired electrons) and (-1 + 1) = 0 respectively.

c) Species having unpaired electrons in both mixed alignment (↑)(↓)

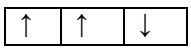
In this case spin multiplicity = [(+n) + (-n) + 1]

where, n = number of unpaired electrons in each alignment. Here, (+ve) sign and (–ve) sign indicate upward and downward alignment respectively.



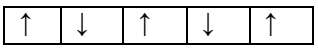
Here total no of unpaired electrons = 2 in which one having upward direction (+1) and other having downward mode (-1).

Hence Spin multiplicity = [(+n) + (-n) +1] = [(+1) + (-1) + 1] = 1 (spin state = singlet)



Here the total no of unpaired electrons = 3 in which two unpaired electrons lie in upward (+2) and one unpaired electrons lie in downward (-1) .

Hence Spin multiplicity = [(+n) + (-n) + 1] = [(+2) + (-1) + 1] = 2 (spin state = doublet)



Here the total no of unpaired electrons = 5 in which three unpaired electrons lie upward (+3) and two unpaired electrons lie downward (-2).

Hence Spin multiplicity = [(+n) + (-n) + 1] = [(+3) + (-2) +1] = 2 (spin state = doublet)

Table 7: (Spin multiplicity and corresponding Spin State)

Number of unpaired electrons (n)	Spin multiplicity value (n + 1)	Spin state
0	1	Singlet
1	2	Doublet
2	3	Triplet
3	4	Quartet
4	5	Quintet
5	6	Multiplet

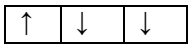
Problems on spin multiplicity and spin state:

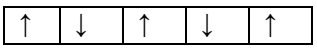
Q.1. Which one of the following will have spin multiplicity value 1 ?

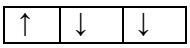
a. B_2 b. B_2^+ c. B_2^- d. B_2^{2-}

Ans: d.B_2^{2-} (Total electrons 12, number of unpaired electrons=0,spin multiplicity= n + 1 = 0 + 1= 0)

Q.2. Which one of the following electronic representation will have zero spin multiplicity value

a. 

b. 

Ans: a.  Spin multiplicity = [(+n) + (-n) + 1] = [+1 – 2 + 1] = 0

Q.3. Which one of the following molecules or ions will have triplet spin state ?

a. NO b. CO c. NO^+ d. NO^-

Ans: d. NO^- (Total electrons = 16, Unpaired electrons, n = 02
spin multiplicity = +n + 1 = +2 + 1 = 3, spin state = triplet)

VI. Calculating of Chemical Bonds (π-Bonds, σ-Bonds, Single and Double Bonds) in Open Chain and Cycloalkene Systems

The molecular formula which defines a very large number of chemical structure, in this particular case, it is a herculean task to calculate the nature and number of bonds. Earlier Badertscher *et al* studied a novel formalism to characterize the degree of unsaturation of organic molecules. But no such work has not been taken till now to calculate the number and types of bonds in open chain olefinic system having complex molecular formulae like $C_{176}H_{250}$, $C_{2000}H_{2000}$.

Keeping this in view, a rapid innovative method has been proposed for the calculation of number of π-bonds, σ-bonds, single and double bonds with the help of following 06 (six) completely new formulae for certain aliphatic unsaturated open chain and cyclic olefinic hydrocarbons.

a) For Open Chain Aliphatic Hydrocarbons

i. *Calculation of π-bonds and double bonds (P)*

The number of π bonds or double bonds for a straight chain olefin is

$$P = [(2X-Y)/2] + 1$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and P = number of π bonds/double bonds.

E.g.: In $C_{176}H_{250}$, X = 176, Y = 250, therefore P = (2 x 176 – 250)/2 +1 = 51 + 1 = 52 number of π bonds or double bonds.

ii. *Calculation of σ-bonds (S)*

The number of σ bonds for a straight chain olefin is

$$S = [X + Y - 1]$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and S = number of sigma bonds (σ-bonds).

E.g.: In $C_{176}H_{250}$, X = 176, Y = 250, therefore P = 176 + 250 -1 = 425 σ bonds.

iii. *Calculation of Single bonds (A)*

The total number of single bond for a straight chain olefin is

$$A = [(3Y/2)-2]$$

where A = number of single bonds and Y is number of hydrogen atoms.

E.g.: In $C_{176}H_{250}$, Y = 250, therefore A = [(3 x 250)/2] = 375 -2 = 373 single bonds. Examples have been illustrated in Table-8.

b) For Cyclic aliphatic olefinic hydrocarbons

i. *Calculation of π-bonds and double bonds (P_c)*

The number of π bonds or double bonds for an aliphatic cyclic olefin is

$$P_c = [(2X-Y)/2]$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and P_c = number of π bonds or double bonds in the cyclic olefinic system.

E.g.: In cyclooctatetraene (C_8H_8), X = Y = 8, therefore P_c = 16-8/2 = 4 number of π bonds or double bonds.

ii. *Calculation of σ-bonds (S_c)*

The number of σ bonds for an aliphatic cyclic olefin is S_c = [X + Y]

Where, X = number of carbon atoms; Y = number of hydrogen atoms and S_c = number of sigma bonds (σ- bonds) in cyclic olefinic system.

Eg: In cyclooctatetraene (C_8H_8), X = Y = 8, therefore S_c = 8+8 = 16 number of σ bonds.

iii. *Calculation of Single bonds (A_c)*

The total number of single bonds in aliphatic cyclic olefin can be calculated by using the formula A_c = [3Y/2]

Where, A_c = number of single bonds and y is number of hydrogen atoms in aliphatic cyclic olefin.

E.g.: In cyclooctatetraene (C_8H_8), Y = 8, therefore A_c = 24/2 = 12 number of single bonds. Examples have been illustrated in Table-9.

Table 8: Calculation of bonds in open chain olefinic hydrocarbons

Example (C_xH_y)	Straight-chain Structure	π bond/ bonds [(2X-Y)/2+1]	σ bonds [X+Y-1]	Single bonds [(3Y/2)-2]	Double bond/bonds [(2X-Y)/2 + 1]
C_2H_4	$H_2C=CH_2$	1	5	4	1
C_3H_6	$H_2C=CH-CH_3$	1	8	7	1
C_3H_4	$H_2C=C=CH_2$	2	6	4	2
C_4H_8	i)$H_2C=CH-CH_2-CH_3$ ii)$H_3C-HC=CH-CH_3$	1	11	10	1
C_4H_6	i)$H_2C=C=CH-CH_3$ ii)$H_2C=CH-CH=CH_2$	2	9	7	2
C_4H_4	$H_2C=C=C=CH_2$	3	7	4	3
$C_{176}H_{250}$	-	52	425	373	52
$C_{2000}H_{2000}$	-	1001	3999	2998	1001
$C_{99}H_4$	-	98	102	4	98

Table 9: Calculation of Bonds in Cyclo Alkene System

Example (C_xH_y)	Cycloalkene	π bond / bonds (P_c) = [(2X-Y)/2]	σ bonds (S_c) [X+Y]	Single bonds (A_c) [(3Y/2)]	Double bond/bonds [(2X-Y)/2]
C_3H_4	Cyclopropene	1	7	6	1
C_4H_4	Cyclobutadiene	2	8	6	2
C_5H_6	Cyclopentadiene	2	11	9	2
C_6H_8	Cyclohexadiene	2	14	12	2
C_7H_8	Cycloheptatriene	3	15	12	3
C_8H_8	Cyclooctatetraene	4	16	12	4

VII. Calculation of π-Bonds, σ-Bonds, Single and Triple Bonds in Straight Chain Alkyne and Cycloalkyne Systems

The number and types of bonds in open chain and cycloalkynes having complex molecular formula is a Herculean task. Keeping this in view, a rapid innovative method has been proposed for the calculation of number of π-bonds, σ-bonds, single and triple bonds with the help of following 08 (eight) completely new formulae by just manipulating the number of carbon and hydrogen atoms by using some factors for certain aliphatic unsaturated open chain and cycloalkynes.

a) Open Chain Aliphatic Alkynes

i. *Calculation of π-bonds (P)*

The number of π bonds for an aliphatic open chain alkyne, where there is one or more than one triple bonds is P= [{(2X-Y)/2} + 1]

Where, X = number of carbon atoms; Y = number of hydrogen atoms and P = number of π bonds.

E.g.: In $C_{16}H_{30}$, X = 16, Y = 30, therefore P = [{(2X-Y)/2} + 1] = [{(2 x 16 – 30)/2} +1] = 2 number of π bonds.

ii. *Calculation of σ-bonds (S)*

The number of σ bonds for an aliphatic open chain alkyne, where there is one or more than one triple bonds is S= [X+Y-1]

Where, X = number of carbon atoms; Y = number of hydrogen atoms and S = number of σ bonds.

E.g.: In $C_{16}H_{30}$, X = 16, Y = 30, therefore, S= [X+Y-1] = [16+30-1] = 45 numbers of σ bonds.

iii. *Calculation of Single bonds (A)*

The total number of single bond for an aliphatic open chain alkyne, where there is one or more than one triple bonds is A = [{(2X+5Y)/2} - 3]/2

Where, A = number of single bonds, X = number of carbon atoms and Y = number of hydrogen atoms.

E.g.: In $C_{16}H_{30}$, X = 16, Y = 30, therefore, A = [{(2X+5Y) / 2} - 3]/2

= [{(2x16+5x30)/2}-3]/2 = [91-3]/2

= 44 numbers of single bonds.

iv. *Calculation of Triple bonds (T)*

In the first case, we have to count the number of carbon atoms (X) and the number of hydrogen atoms (Y) in a given unsaturated hydrocarbon containing triple bonds. The formula to calculate the number of triple bonds for an aliphatic open chain alkyne, where there is one or more than one triple bonds is

$$T= [\{(2X-Y)/2\} + 1]/2$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and T = number of triple bonds.

E.g.: In $C_{16}H_{30}$, X = 16, Y = 30, therefore, T = [{(2X-Y)/2} + 1]/2

= [{(2 x 16 – 30)/2} +1]/2

= 2/2 = 1 triple bond.

Examples have been illustrated in Table-10.

b) Cycloalkynes

i. *Calculation of π-bonds (P_c)*

In the first case, we have to count the number of carbon atoms (X) and the number of hydrogen atoms (Y) in the given unsaturated cycloalkyne.

The number of π bonds for an aliphatic cycloalkyne is

$$P_c= [(2X-Y)/2]$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and P_c = number of π bonds in the cycloalkyne system.

E.g.: In Cycloheptyne (C_7H_{10}), X =7, Y = 10, therefore P_c = (2x7-10)/2 = 2 number of π bonds.

ii. *Calculation of σ-bonds (S_c)*

The number of σ bonds for an aliphatic cycloalkyne is

$$S_c = [X + Y]$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and S_c = number of sigma bonds (σ-bonds) in cyclo alkyne system.

E.g.: In Cycloheptyne (C_7H_{10}), X =7, Y = 10, therefore S_c = (7+10) = 17 number of σ bonds.

iii. *Calculation of Single bonds (A_c)*

The total number of single bond for an aliphatic cycloalkyne is

$$A_c = [\{(2X+5Y)/2\}]/2$$

Where, A_c = number of single bonds in cycloalkyne, X = number of carbon atoms and Y = number of hydrogen atoms.

E.g.: In Cycloheptyne (C_7H_{10}), X = 7, Y = 10, therefore, A_c = [{(2X+5Y)/2}]/2

= [{(2x7+5x10)/2}]/2=32/2 = 16 numbers of single bonds.

iv. *Calculation of Triple bonds (T)*

The number of triple bond is T_c= [{(2X-Y)/2}]/2

Where, X = number of carbon atoms;

Y = number of hydrogen atoms and

T_c = number of triple bond.

E.g.: In Cycloheptyne (C_7H_{10}), X =7, Y = 10, therefore, T_c = [{(2X-Y)/2}]/2 = [{(2 x 7 – 10)/2}]/2 = 2/2 = 1 triple bond.

Table 10: Calculation of bonds in open chain Alkyne system)

Example for Open Chain Alkyne (C_xH_y)	π bonds [{(2X-Y)/2} + 1]	σ bonds [X+Y-1]	Single bonds [{(2X+5Y)/2} - 3]/2	Triple bond/bonds [{(2X-Y)/2} + 1]/2
$C_{10}H_{18}$	2	27	26	1
$C_{11}H_{20}$	2	30	29	1
$C_{12}H_{22}$	2	33	32	1
$C_{13}H_{24}$	2	36	35	1
$C_{14}H_{26}$	2	39	38	1
$C_{15}H_{28}$	2	42	41	1
$C_{16}H_{30}$	2	45	44	1
C_6H_6	4	11	9	2
$C_{12}H_{14}$	6	25	22	3

IV. Conclusions

It may be expected that these innovative methods would go a long way to help to the students of chemistry at Undergraduate, Senior Undergraduate and Post-Graduate level who would choose the subject as their career. Experiment *in vitro* on 100 students showed that by using these new innovative methods students can save up to 30-40 mins time in the examination hall. On the basis of this, I can strongly recommend to use these new time economic interesting pedagogies.

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Chemical Concepts Inventory: Correlates between the Acquired Level of Knowledge and the Positive Attitudes toward the Concept

By Kallistheni A. Georgiou, Miltiades A. Kyprianou
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Abstract- The current study undertakes, through a structured Chemical Concepts Inventory (CCI), to evaluate the level of understanding of 15-year old Greek students of chemical ideas focused around the central concept of the periodic system of chemical elements. At the same time, using a Semantic Differential Scale Questionnaire, the study appraises the students' attitude toward the periodic system. As a corollary to the above the study hypothesized the existence of collaterality between high grades and positive attitudes. The two questionnaires were administered to 103 students from two schools after the completion of the relevant syllabus in 26 weeks. Results showed that the scores in the CCI largely follow the same distribution, central tendency and dispersion as school tests and exams.

Keywords: chemical education research, chemical concepts inventory, attitude toward chemistry, semantic differential.

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Chemical Concepts Inventory: Correlates between the Acquired Level of Knowledge and the Positive Attitudes toward the Concept

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Abstract- The current study undertakes, through a structured Chemical Concepts Inventory (CCI), to evaluate the level of understanding of 15-year old Greek students of chemical ideas focused around the central concept of the periodic system of chemical elements. At the same time, using a Semantic Differential Scale Questionnaire, the study appraises the students' attitude toward the periodic system. As a corollary to the above the study hypothesized the existence of collaterality between high grades and positive attitudes. The two questionnaires were administered to 103 students from two schools after the completion of the relevant syllabus in 26 weeks. Results showed that the scores in the CCI largely follow the same distribution, central tendency and dispersion as school tests and exams. There is a significant decrease of the scores as the syllabus moves through the four units (structure of the atom, electronic orbitals, periodic table and chemical bonds), which may be attributed to the increasing difficulty of the scientific ideas coupled with disproportionate time allocated for their assimilation. The students' attitude toward the periodic system was largely positive. Scores in the CCI were significantly and positively correlated with in the semantic differential scores, thus substantiating the working hypothesis. This means that the semantic importance attributed to the concept of the Periodic System is directly related to the level of knowledge acquired by the student in chemistry. In a more general context, the conceptual importance attributed to a science discipline is related to the level of cognition attained in the specific discipline.

Keywords: chemical education research, chemical concepts inventory, attitude toward chemistry, semantic differential.

Graphical abstract

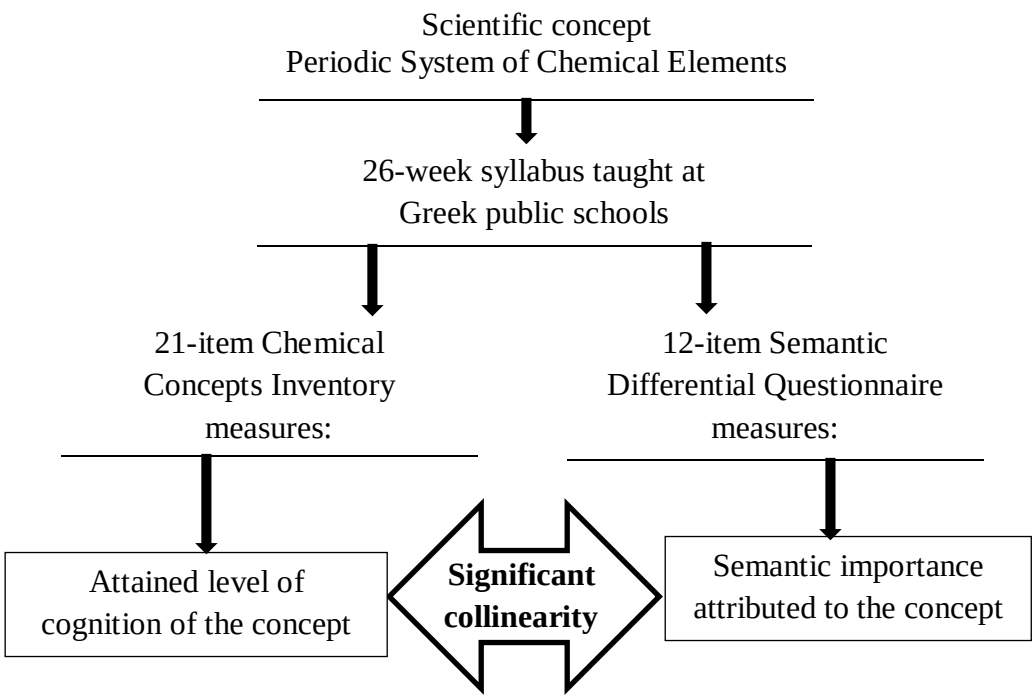

Figure 1

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I. Introduction

A concept inventory (CI) can be defined as a test, usually in multiple-choice form, designed to determine how well students have assimilated the basic concepts of a discipline they have been taught for the first time. Historically the first CI to appear was the Force Concept Inventory (FCI).[1,2] The FCI covers the basic physics syllabus: kinematics, Newton's First, Second and Third Laws, superposition principle and kinds of forces with special attention to gravitation. There followed CIs for several other disciplines and subdisciplines. In chemistry several CIs have been developed, each one reflecting the relevant syllabus taught.[3,4]

Being a questionnaire, every CI evidently entails its own psychometric properties, especially with regards to reliability and validity.[5]Beyond this, every concept taught invariably invokes specific reactions from the recipient, who will eventually form his own attitudes towards the concept whether they be conscious or subconscious. These attitudes can be evaluated by using semantic differential techniques.[6,7]It has been argued that, in contrast to Likert-based response formats, "in measuring positive psychological constructs, a semantic differential format may effectively reduce acquiescence bias without lowering psychometric quality".[8]

In fact, a 20-item semantic differential instrument to measure student attitudes toward the subject of chemistry (ASCI) has already been developed and tested.[9] Subsequently a shortened version (ASCIv2) was developed and validated, which substantiated a two-factor structure of the instrument measuring intellectual and emotional attitudes.[10]

There remains the question whether the attitudes towards the concept would be correlated to the scores obtained in the inventory. In a meta-analysis regarding public understanding of science the authors found a "small positive correlation between general attitudes towards science and general knowledge of scientific facts".[11] However, the same approach has not been applied with regards to concept inventories.

In view of the above the current study focused on the following three goals: First, to develop and test a structured Chemical Concepts Inventory, to evaluate the level of understanding of 15-year old Greek students of chemical ideas focused around the central concept of the periodic system of chemical elements. Second, using a Semantic Differential Scale Questionnaire, to appraise the students' attitude toward the periodic system. Third, to test the hypothesis of the existence of a strong link between a subject's positive attitude towards a concept and his/her comprehension of its main ideas

II. Methods

Questionnaires

The current study utilizes two questionnaires. The first is the Chemistry Concept Inventory (CCI) and the second is the Semantic Differential Scale Questionnaire (SDSQ). The CCI (see Supporting Information, Part A) contains 21 multiple choice questions that cover the chemistry syllabus taught during the first semester of the first year in Greek Public Lyceums, supervised by the Greek Ministry of Education. The 45-minute classes cover the span of 26±1 weeks with 2 lessons per week. The syllabus and accordingly the inventory are centered on the fundamental concept of the periodic system of elements and are divided into four units, taught in the order: structure of the atom (5), electronic orbitals (4), periodic table (7) and chemical bonds (5). In parentheses are the numbers of questions in the inventory that refer to each section. The questions that pertain to each section and the correct answers are shown in Supporting Information Part A.

The second instrument was the Semantic Differential Scale Questionnaire (SDSQ) containing twelve dipoles, aiming at measuring the students' attitude towards the Periodic System. The wording of the questionnaire and the dipoles used are included in Supporting Information, Part B.

Both the semantic questionnaire and the Chemistry Concept Inventory (CCI) were given upon the completion of the syllabus during the last week of January 2015. One important nuance of the experimental procedure is that the Semantic differential scale questionnaire and the Chemistry Concept Inventory (CCI) were given in this order, so that the subject's conception of his/her performance in the inventory might not interfere with his/her attitude towards the concept.

The sample of 103 students came from two Greek public schools (lyceums), one in Athens and one in Piraeus. One school was an experimental school. The School X Gender cross tabulation is shown in table 1.

Table 1: School X Gender cross tabulation of the students

	Gender		
School	Male	Female	Total
Athens	25	28	53
Piraeus	34	16	50
Total	59	44	103

III. Statistical Analysis

The CCI was subjected to rigorous analysis, reporting the basic characteristics of the distribution, central tendency and dispersion of the total scores, which were further subjected to two-factor analysis of

variance (ANOVA) with gender and school (and their interaction) as the between subjects factors. The four section scores were subjected to ANOVA with repeated measures followed by post-hoc pairwise comparisons with Bonferroni corrections. The twelve semantic differential scores were tested if they differed significantly from zero with the one-sample t-test, as well as with ANOVA with repeated measures. Subsequently the twelve scores were subjected to factor analysis and the results were compared to the results of the above ANOVA procedure. Finally, the associations between the scores from the two questionnaires were established with the use Pearson's correlation coefficients. The level of significance was set at 0.05.

IV. Results

a) Chemistry Concepts Inventory (CCI)

The box plot and histogram of the frequency distribution of the students' score in CCI (Figure 2) summarize the basic characteristics of the distribution, central tendency and dispersion of the scores in CCI. The fact that the mean of 49.7 (SD=18.8) is very close to the median of 48 is indicative of a normal distribution. This is corroborated by the likeness of the distribution to the normal curve and confirmed by Kolmogorov-Smirnov test (p=0.126).

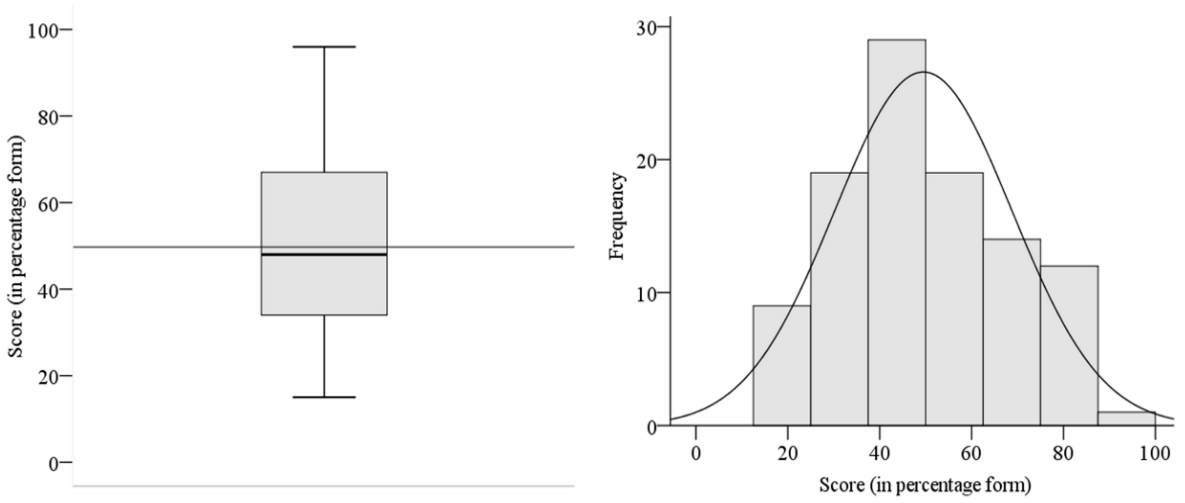

Figure 2: Boxplot and histogram of the frequency distribution of the students' score in CCI

The ANOVA model proved that the CCI score is independent from gender (p=0.222), school (p=0.482) and their interaction (p=0.257). However the repeated measures ANOVA revealed that the average section scores in percentage form (Figure 3) differed significantly ($F(3,306)=23,3$, $p<0.01$). Post-hoc pairwise comparisons with Bonferroni corrections proved that the average score in the chemical bonds section was significantly lower ($p<0.01$) than in the three other sections. Significantly lower ($p<0.01$) was also the average score in the periodic table section in comparison to the structure of the atom section.

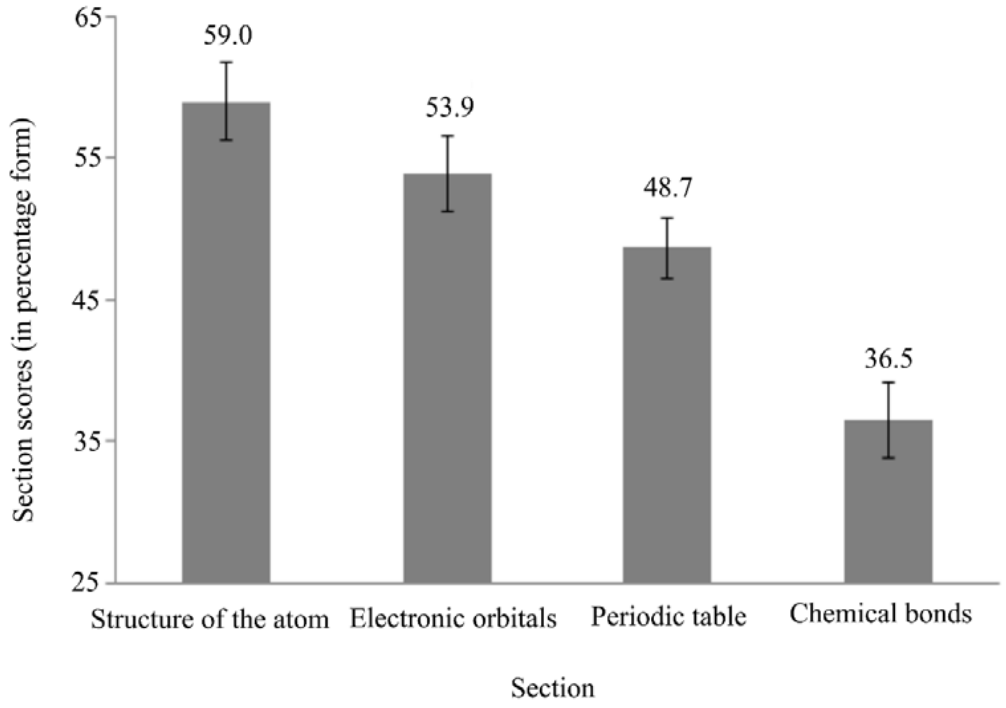

Figure 3: Mean values with standard errors of the scores in the four sections of CCI

b) Semantic Differential Scale Questionnaire (SDSQ)

Figure 4 shows the mean values and standard errors of the scores in the twelve semantics used in the current questionnaire. Overall the students gave a positive score to the notion of the Periodic Table. For nine out of the twelve concepts the score was significantly greater than zero ($p<0.05$). The scores for two concepts (sweet and young) did not differ from zero, while for the concept of noisy it was significantly less than zero. Probably for this concept it is better to reverse the scores.

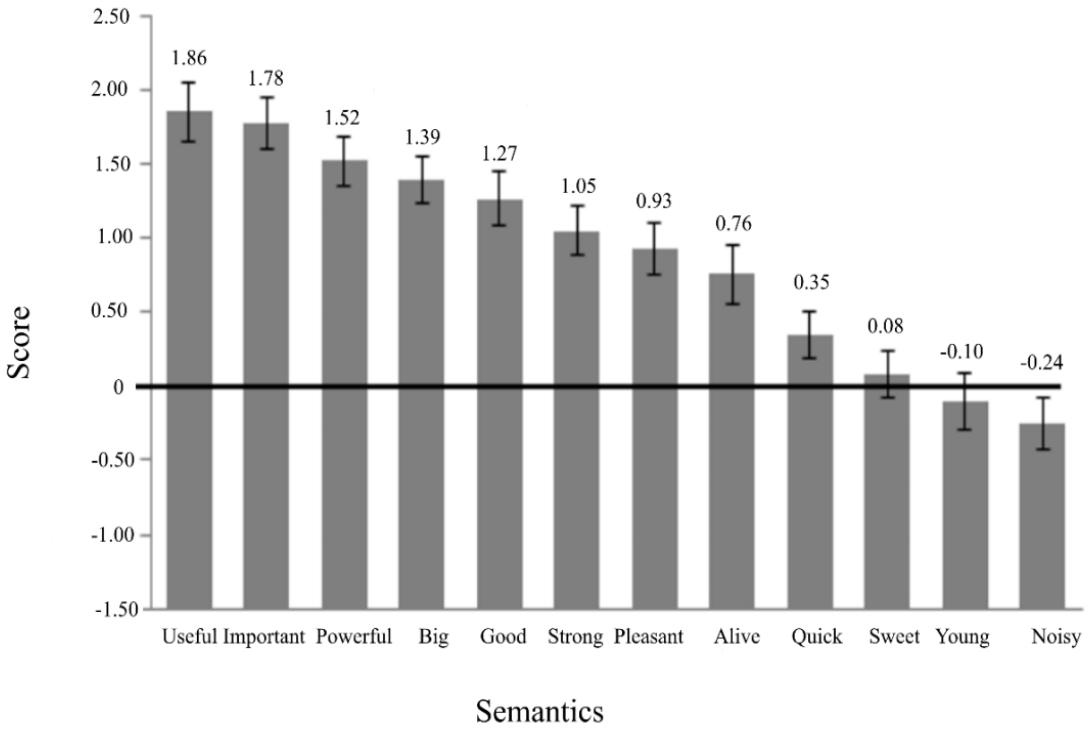

Figure 4: Mean values and standard errors of the scores in the twelve semantics

It is obvious that there were significant differences between the mean scores in the twelve concepts ($F(3,306)=23.3$, $p<0.01$). As figure 3 shows, there was a group of six concepts from useful to strong, where the mean score was greater than one.

Table 2 shows the results of the application of exploratory factor analysis on the scores of the twelve concepts. There were three factors extracted with eigenvalues greater than one, explaining 65.3% of the total variability. Most interesting is the first factor with an eigenvalue of 3.7 that explains 30.6% of the total variability. The factor is composed of the six concepts that received the highest mean score, as shown above. Moreover, the loadings of the concepts follow the same patterns with their mean scores.

Table 2: Loadings of the concepts on the three extracted factors, shown with their eigen values and proportion of variance explained

Concept	Factor		
	1	2	3
Useful	0.857		
Important	0.833		
Powerful	0.794		
Strong	0.681		
Big	0.675		
Good	0.627		
Sweet		0.824	
Alive		0.705	
Pleasant		0.674	
Young		0.570	
Noisy			0.867
Quick			0.619
Eigenvalue	3.7	2.7	1.4
% of variance	30.6%	22.8%	12.0%

Consequently, both approaches point to the same conclusion that from the total of the twelve semantic (conceptual) dipoles, six of them imprint the positive attitude of the students towards the notion of the Periodic Table. Therefore, the first factor conceptualizes the positive attitudes to the construct of the Periodic Table, while the second and third factors respectively encompass the neutral and negative attitudes.

c) *Correlation between scores in Chemistry Concept Inventory and Semantic Differential Scale Questionnaire*

Table 3 shows the Pearson's correlation coefficients between the twelve scores in the Semantic Differential Scale Questionnaire and the total score and the scores in the four sections of the Chemistry Concept Inventory. The total score is significantly correlated with six out of the twelve semantic dipoles. The interesting detail is that five out of the six significant correlations are with the concepts with the highest score that are constituents of the first factor. The only differentiation is the absence of significant correlation with the semantic dipole big-small and the presence of significant correlation with the dipole sweet-sour.

Table 3: Pearson's correlation coefficients between the scores in differential semantics and the total score and the scores in the four sections of the Chemistry Concept Inventory

Concept	Total score	CCI scores Structure of the atom	Electronic orbitals	Periodic table	Chemical bonds
Important	0.358**	0.355**	0.319**	0.254*	0.148
Useful	0.300**	0.261**	0.252*	0.209*	0.176
Strong	0.292**	0.316**	0.230*	0.193	0.132
Powerful	0.244*	0.279**	0.064	0.217*	0.137

Good	0.231*	0.315**	0.183	0.126	0.069
Sweet	0.202*	0.251**	0.217*	0.172	-0.035
Young	0.185	0.326**	0.226	0.050	-0.039
Alive	0.174	0.306**	0.188	0.069	-0.037
Pleasant	0.172	0.280**	0.092	0.111	0.019
Quick	0.150	0.238*	0.045	0.113	0.030
Big	0.139	0.150	0.069	0.075	0.119
Noisy	0.105	0.145	0.036	0.077	0.054

** - *Correlation is significant at the 0.01 level*

* - *Correlation is significant at the 0.05 level*

Moreover, as table 3 shows, semantic relevance is significantly associated with the scores in the section of the structure of the atom, where there were ten significant correlations. The number of significant correlations drops in subsequent sections concomitantly with the drop in the scores of corresponding sections. Thus there were only four significant correlations of semantic concepts with the score in the section of electronic orbitals, two with the score in the section of the periodic table and none with the score in the section of chemical bonds.

V. Discussion

The current study undertakes, with the use of a Chemical Concepts Inventory, to evaluate the level of knowledge and understanding of the basic concepts built around the Periodic System of Chemical Elements attained by 15-year old Greek students who are taught the discipline for the first time. At the same time, using a Semantic Differential Scale Questionnaire, the study appraises the students' attitude toward the concept of the Periodic Table. The most notable finding hereof is that the level of understanding is concomitant with more positive attitude towards the concept.

The scores in the Chemical Concepts Inventory largely follow the same distribution, central tendency and dispersion as school tests and exams. The fact that there is a significant decrease of the students' score as the syllabus moves through the four units (structure of the atom, electronic orbitals, periodic table and chemical bonds) could be explained by two pivotal points. Firstly, the underlying concepts of the units gradually increase in complexity, requiring at the same time the basic understanding of the concepts of the previous units. Secondly, as the teacher is well aware of the above fact, he will probably try to teach the lesson without leaving any gaps, which may in the end result that the later more difficult units will be taught in a disproportionately less time than the one required. As a consequence, the student's understanding of the very important concepts of chemical bonds, as reflected by their corresponding scores in the inventory, leaves much to be desired.

The results of the semantic differential scale questionnaire showed that, overall the students had a positive attitude towards the concept of the Periodic Table. In point of fact the semantics that did not receive a significant positive score are represented by dipoles that bear practically no relevance of an attitude towards a scientific concept.

The most interesting finding is the presence of significant positive correlation between the scores in the Chemical Concepts Inventory and the scores in the Semantic Differential Scale Questionnaire. Even more fascinating is that this association is stronger with concepts that the students had higher scores, i.e. concepts that are more understandable to the students. This means that the semantic importance attributed to the concept of the Periodic System is directly related with the level of knowledge acquired by the student in chemistry. This finding is in agreement with previously published research evidencing that attitude and achievement are related.[12,13]

The above conclusion can be reworded in a more generalized context: The conceptual importance attributed to a science discipline is related to the level of cognition attained in the specific discipline. In other words, "the more I understand it, the more I like it". Perhaps, even this relationship is bidirectional.

VI. Limitations

The scores of the CCI presently presented clearly reflect the knowledge level attained by the students in Greek public schools as per the syllabus taught and its time limits according to the guidelines of the Greek Ministry of Education.

VII. Implications

This pilot study has pointed to the potential of building and fine-tuning the teaching of the chemical discipline with critical awareness about the curriculum terminology in ways based on interactive support which draws on the principle of "guidance through interaction in context of shared experience".[14]

Our conjectures remain tentative and our findings more promising than decisive. However, using the perspective of semantic meaning in classroom pedagogies appears to offer not only ways of understanding, but, just as importantly, to demystify the structuring of knowledge in chemical discipline in ways that may enable more students to succeed.

Furthermore, the use of semantic meaning methodology provides a tool for studying intangible knowledge regarding the learner's understanding that are often hard to discern with other methods. This approach also allows better control of intervening variables than classroom-based research.

VIII. Associated Content

a) Supporting Information

It includes the content of the two questionnaires: the Chemistry Concept Inventory (CCI) and the second is the Semantic Differential Scale Questionnaire (SDSQ).

i. *The Chemistry Concepts Inventory (CCI)*

a. Questions

For each question circle the letter that you believe corresponds to the right answer.

Choose only one answer for each question.

Please do not leave unanswered questions.

Try to avoid guessing. Your answers should be indicative of your own personal way of thinking.

Try to complete the test within 20 minutes.

Your performance in this inventory will have no consequences in your final grade in the chemistry lesson.

Thank you for your cooperation.

1. In the nucleus of an atom there are:
A. Only electrons and protons
B. Only neutrons
C. Only electrons and neutrons
D. Electrons, protons and neutrons
E. Only neutrons and protons

2. In a neutral atom always:
A. The number of electrons is equal to the number of neutrons
B. The number of electrons, protons and neutrons is equal
C. The number of electrons is equal to the number of protons
D. The number of neutrons is equal to the number of protons
E. None of the above

3. The identity of an atom is:
A. Its mass number
B. Its atomic number
C. Its number of neutrons
D. Its number of electrons and neutrons
E. None of the above

4. Isotopes are elements that have:
A. The same mass number and the same atomic number
B. The same mass number
C. Different mass numbers and the same atomic number
D. Different atomic numbers and the same mass number
E. None of the above

5. In an atom of an element there are 20 neutrons and there is one neutron more than there are protons. Its mass number is:
A. 1
B. 19
C. 20
D. 21
E. 39

6. When an electron of a neutral atom jumps from an inner to an outer orbital:
A. The atom converts into a cation
B. The atom converts into an anion
C. Energy is released
D. Energy is absorbed
E. The atom remains at the same energy state

7. The atom of a neutral atom loses an electron. The atom:
A. Converts into a cation
B. Converts into an anion
C. Remains as it is
D. Changes its mass number
E. Changes its atomic number

8. The atom of calcium has the atomic number 20. In its fundamental state on the outer orbital the atom has:
A. No electrons
B. 1 electron
C. 2 electrons
D. 8 electrons
E. 10 electrons

9. Chlorine has the electron configuration (2, 8, 7). In order to attain the structure of a noble gas it must:
A. Gain a proton
B. Lose a proton
C. Lose an electron
D. Gain an electron
E. Gain a neutron

10. Two elements have similar chemical properties. These two elements:
A. Belong to the same group of the periodic table
B. Belong to the same period of the periodic table
C. Have the same number of neutrons
D. Have the same mass number
E. Have the same atomic number

11. The chemical elements in a period of the periodic table have the same number of:
A. Protons in the nucleus
B. Electron orbitals
C. Electrons in the nucleus
D. Electrons in the outer orbital
E. Neutrons in the nucleus

12. In an aqueous solution of sodium chloride there are:
1. Sodium chloride molecules
2. Sodium and chlorine atoms
3. Sodium cations and chlorine anions
4. Sodium anions and chlorine cations
5. Sodium cations and chlorine atoms

13. The bond in the oxygen molecule is:
A. Ionic
B. Nonpolar simple covalent
C. Polar double covalent
D. Nonpolar double covalent
E. Nonpolar triple covalent

14. The chemical elements $_{12}A$ and $_{9}B$ form an ionic compound with the chemical formula:
A. AB
B. A_2B
C. A_2B_2
D. B_2A
E. AB_2

15. The chemical elements $_{3}Li$, $_{11}Na$ and $_{19}K$ have in the order they are given:
A. Increasing atomic radius and increasing electropositivity
B. Decreasing atomic radius and increasing electropositivity
C. Increasing atomic radius and decreasing electropositivity
D. Decreasing atomic radius and decreasing electropositivity
E. Increasing atomic radius and the same electropositivity

16. Across the same period the atomic radius:
A. Increases
B. Decreases
C. remains the same
D. at first increases and then decreases
E. at first decreases and then increases

17. The oxidation number of the atom of Nin the molecule of N_2 is
A. -1
B. 0
C. +1
D. -3
E. +3

18. The oxidation number of S in Na_2SO_4 is:
A. -6
B. -2
C. 0
D. +2
E. +6

19. In which part of the periodic table are the nonmetals?
A. In the middle
B. In the right part
Γ. In the left part
Δ. In the upper part
E. In the lower part

20. Which category comprises the majority in the periodic table?
A. The metals
B. The metalloids
C. The nonmetals
D. The noble elements
E. The lanthanides

21. The atom of element A has two electrons at the outer orbital of element B has 7. In which groups do these elements belong?
A. Alkali metals and alkaline earths
B. Halogens and noble gases
C. Halogens and alkali metals
D. Alkaline earths and halogens
E. Alkali metals and noble gases

b. Correct answers

Question	1	2	3	4	5	6	7	8	9	10	11
Answer	E	C	B	C	E	D	A	C	D	A	B
Question	12	13	14	15	16	17	18	19	20	21	
Answer	C	D	E	A	B	B	E	B	A	D	

c. Sections

Structure of the atom (5)	1, 2, 3, 4, 5
Electronic orbitals (4)	6, 7, 8, 9
Periodic table (7)	10, 11, 15, 16, 19, 20, 21
Chemical bonds (5)	12, 13, 14, 17, 18

i. *Semantic Differential Questionnaire*

The perception of the significance of a concept is accompanied by its agreement or disagreement (relative or absolute) with other concepts. In this context we would like you to try to imprint the degree of your agreement (or disagreement) in reference to the importance of the concept of the PERIODIC SYSTEM of elements in Chemistry in relation to the semantic dipoles that follow.

For each dipole circle the number that best suits your attitude. If you are not certain give the most probable answer.

The present grading refers to the relation that you a scribe, of the importance of the concept of the PERIODIC SYSTEM with the semantic dipoles that follow, at present after the completion of the educational program.

Pleasant	3	2	1	0	1	2	3	Unpleasant
Big	3	2	1	0	1	2	3	Small
Fast	3	2	1	0	1	2	3	Slow
Good	3	2	1	0	1	2	3	Bad
Strong	3	2	1	0	1	2	3	Weak
Alive	3	2	1	0	1	2	3	Dead
Sweet	3	2	1	0	1	2	3	Sour
Powerful	3	2	1	0	1	2	3	Powerless
Noisy	3	2	1	0	1	2	3	Calm
Useful	3	2	1	0	1	2	3	Useless
Important	3	2	1	0	1	2	3	Trivial
Young	3	2	1	0	1	2	3	Old

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Removal of Toxic Nitrate and Nitrite from Wastewater by Valuarized Fish Scales Waste Remains

By Morlu G. F. Stevens & Bareki S. Batlokwa
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Abstract- In this work, the adsorption efficiency of fishscales was investigated as an environmentally-friendly and cheap alternative sorbent for removing excess nitrate and nitrite from wastewater. The pulverized size of the fishscales was found to be ≤60 μm, with rough surfaces. Multivariate methodology was employed for optimization of parameters that affect sorption; initial ion concentration which were found to be 28.44 mg/L (NO_2^-) and 28.29 mg/L (NO_3^-), the sorbents; 78.48 mg/L (NO_2^-) and 71.17 mg/L (NO_3^-), contact time, which were found to be 65.72 min (NO_2^-) and 74.84 min (NO_3^-), and solution pH 7.97 (NO_2^-) and 7.00(NO_3^-). The optimized adsorption method exhibited high percentage removal efficiencies toward nitrite and nitrate removal from real wastewater samples at 91.42% and 74.60% with a relative standard deviation (RSD) of 1.44% and 2.09% for n = 3 respectively. Physico-chemical characterization of the fishscales showed multiple functional groups including, carboxylic, hydroxyland carbonyls. The adsorption of ions onto valuarized fishscales was endothermic and spontaneous and the adsorption data followed second-order kinetics.

Keywords: *nitrate, nitrite, fishscale waste, adsorption, valuarized waste and wastewater.*

GJSFR-B Classification: *FOR Code: 090499*

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I. Introduction

Nitrate (NO_3^-) and nitrate (NO_2^-) are two different oxidation states of nitrogen (N) that are of environmental health concerns to many researchers [1]because of their solubility nature in water, which has a toxic health effect to humans and aquatic life. The advancement of technology, rapid pace of industrialization, population expansion, agricultural activities and unplanned urbanization contribute to the increased quantities of the two ions thus contaminating surface and ground waters [2]. Nitrate contaminations occur due to the widespread applications of fertilizers containing nitrate for agricultural activities and inadequate treated or untreated human and animal wastes. Nitrate and nitrite have been detected in surface waters, drinking water, ground water and wastewater effluent. Nitrogen exists naturally in soils, typically bounded to organic matter and mineral soil material usually at low concentrations[3]. They also form part of the human diet and can be found in vegetables, fruits, cured meats, fish, dairy products, beers, cereals, and cereal products[4]. However, high level of nitrate concentration in the aquatic environment causes a serious health risk, responsible for methemoglobinemia, decreases in blood pressure, increased heart rate, reduced ability of the blood to carry oxygen to tissues, headaches, abdominal cramps, vomiting, and even death [5].

Reverse osmosis[6], ion exchange[7], powdered activated carbon adsorption[8], the biofilm-electrode reactor (BER),combined membrane bioreactor [9] and adsorption process [1] have been over the past years been employed as conventional removal methods of nitrate and nitrite anions removal from wastewater. However, these methods present some drawbacks, such as high cost and the disposal of the resulting sludge [10].Because of the drawbacks, researchers have turned their attentions to the use of low-cost alternative adsorbents for the removal of nitrate and nitrite anions from wastewater.

In this work, a method employing *valuarized fish scales waste remains* for simultaneously removing toxic nitrate and nitrate anions from wastewater was developed. The study was aimed at developing a cheaper, faster, non-toxic and environmental friendly treatment of wastewater effluent for the removal toxic anions.

II. Materials and Instrumentations

The adsorbent used for the experiments was fish scales waste remains collected from Lake Ngami in Sehitwa, Botswana. Reagents used were: white spirit Vinegar, employed to treat the waste materials, purchased from SPAR (Palapye, Botswana), elemental standard solution of NO_2^-, and NO_3^- with a concentration of 1000 mg/L and NaOH (97%) pellets were purchased from Rochelle Chemicals (Johannesburg, South Africa).A JSM 1700 SEM coupled with EDX, obtained from USA was employed for morphological and elemental analysis. Perkin Elmer System, Spectrum two fourier transform infrared (FTIR)spectroscopy was used to determine the functional groups of materials. ALabRAM HR Evolution Raman S0 – TNO4 Spectrometer (JobinYVon Technology, France) obtained from JobinYVon Technology (Villeneuve d'Ascg, France)

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was employed for characterization of the adsorbents. Meanwhile, nitrate and nitrite anions were determined by a Shimadzu S 150 ion chromatography system (SHIMADZU, Japan) obtained from SHIMADZU (Johannesburg, South Africa).

III. Pre-Treatment of the Fish Scales Waste Remains

The waste remains were washed thoroughly with deionized water to remove mud and unwanted contaminants. After washing the remains, they were sun dried for 48hrs, than pulverized employing a Fritsch pulverisette 5 pulverizer, operated at 400 rpm for 90 min. The pulverized materials were then sieved using 65 – 200 micron mesh size, rewashed with deionized water several times to remove color and dust, and then treated with SPAR white spirit vinegar to remove inorganic pollutants. Finally, they were dried in an oven at 65 ± 5 °C for 6hrs. Characterization of the VFSWR showed the effectiveness of the vinegar during the treatment process (see figures: 1 and 2).

IV. Characterization of Valuarized Fish Scales Waste Remains

To evaluate and reveal details on the physical and chemical properties of the valuarized fish scales waste remains, fourier transform infrared spectroscopy (FT-IR) and scanning electron microscopy coupled with energy dispersive X-ray spectroscopy (SEM-EDX) were employed for the characterization.

Fourier Transform Infrared Spectrometer (FTIR) was employed to investigate the functional groups responsible for analyte interaction with the VFSWR. Figure 1 below shows the functional groups of fish scales before removal (black) and after removal (red) of nitrate and nitrite anions. The functional groups that are prominent in the fish scales are 1016cm-1 due to carboxyl bands and primary amines, 554 to 597 cm^{-1} due to alkanes, 870 cm^{-1} due to sulphonates, -OH and N-H groups at 3286 cm^{-1}, C-O group at 1542.1 to 1642.4 cm^{-1} and C-H, $-CH_3$, $-CH_2$ groups at 1408.4 cm^{-1}

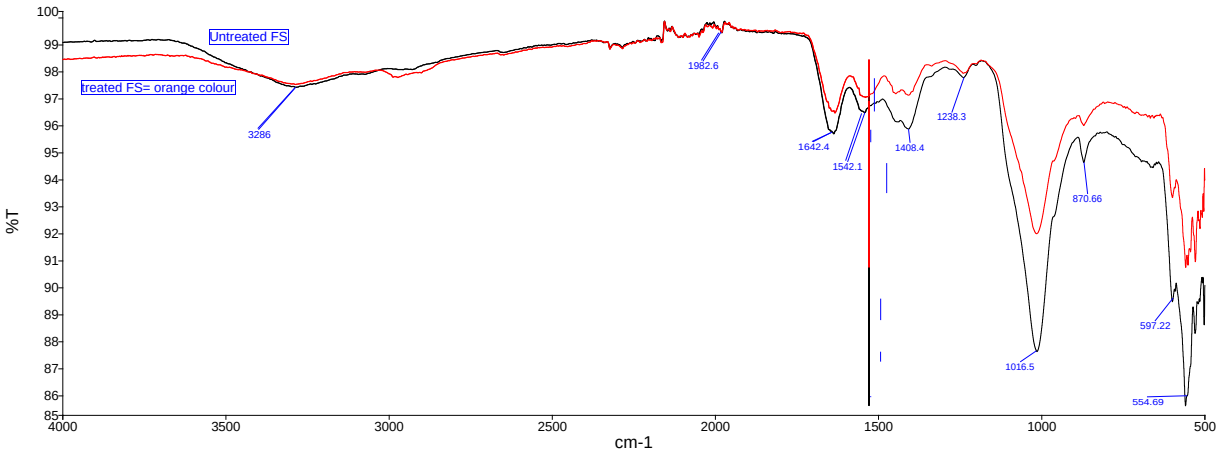

Figure 1: FTIR of fish scales before removal (black) and after removal (red) of target analytes

Fig. 2 shows SEM micrographs of the loaded VFSWR, and VFSWR. The VFSWR as shown in Fig. 2A appears to have a rough surface and are characterized by having two regions, one being darker and the other being white. The white region is rich in inorganic material containing high proportion of calcium and phosphorus whereas the dark region is rich in protein because it has high proportion of carbon and oxygen. From energy, dispersive X-ray (EDX) analysis, inorganic ions were confirmed in the fish scales before valuarization and after adsorption of ions. Figure 2B clearly shows that the presence of new shiny bulky particles over the surface of ions loaded VFSWR which are absent in the VFSWR. These results confirm the binding of ions in fish scale through adsorption.

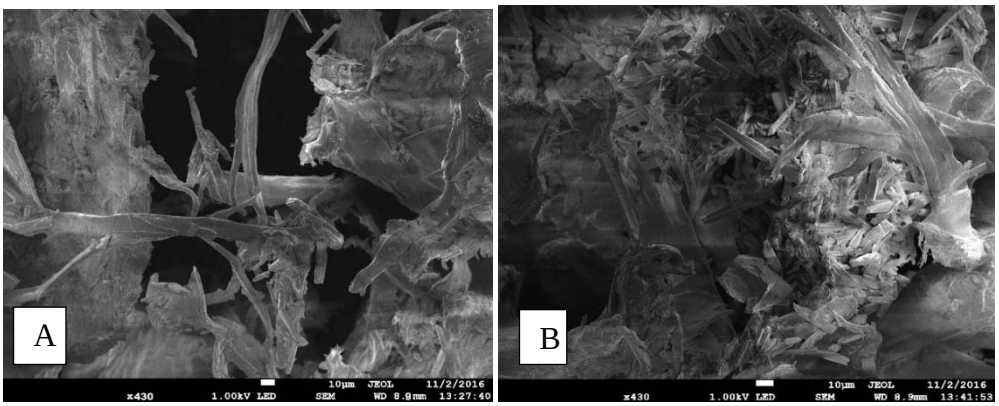

Figure 2: SEM images of the A) VFSWR and B) loaded VFSWR

V. Optimization of Adsorptive Parameters of the Valuarized Fish Scales Waste Remains

Optimization studies were carried out using multivariate optimization methodology. In this study, VFSWRwas optimized by looking at four factors; contact time, pH, VFSWR dosage, as well as concentration. These were first evaluated by employing a two-level fractional factorial design. This design enabled identification of the significance of each factor towards the experimental output. Following this, a face centered central composite design was then performed to determine the optimum conditions for each factor that would result in a maximum response of the experiments. The optimization process was carried out with the use of Minitab Release 14 statistical software (Minitab Inc., USA).

Analysis of the ½ fraction factorial design data was in the forms of normal probability plots of standardized effects as shown by Figures 3. From the normal probability plot of standardized effects, the magnitude of the main effects of each factor as well as the effects brought about by the interaction of factors is represented by its distance from the solid line and the side on which the effect lies with respect to the solid line. Negative effects lie to the left while positive effects lie to the right of the solid line. The solid line indicates where the points would fall if the effects were zero, while the percentage in the y-axis signifies the weight age of each factor's contribution towards the obtained yield. The normal probability plots of standardized effects of NO_2^- showed that there was a significant contribution towards the obtained yield as a result of interaction between factors (Factor A and Factor B), while, that of NO_3^- showed that there was a significant contribution towards the obtained yield as a result of interaction between factors (Factor A and Factor C).

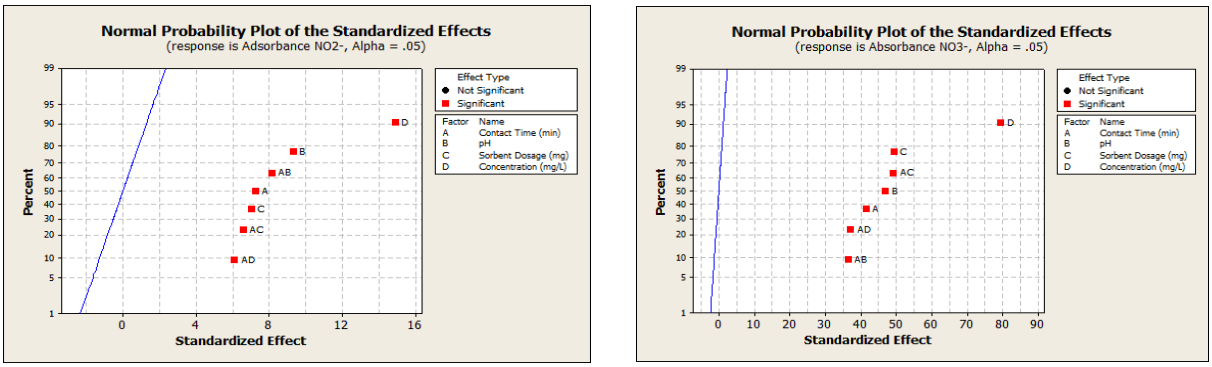

Figure 3: The normal probability plots of standardized effects of nitrite and nitrate for the VFSWR

Table 1: Factors and their levels for the two-level fractional factorial design for the optimization of the VFSWR

Variable	Factor	Low level	High level
A	VFSWR dosage (mg)	25	1000
B	pH	2	10
C	Contact time (minutes)	15	180
D	Concentration (mg/L)	0	50

Response surfaces and the response optimizer were employed to determine the optimum conditions of each factor in relation to the VFSWR. Test for the significance of the quadratic model was done using the F-test for ANOVA at 95% confidence level. The optimal parameters following performance of the experiments are shown in Tables 2.

Table 2: Optimal parameters for adsorptive efficiency of the VFSWR

Anions	pH	VFSWR dose (mg/L)	Contact time (min)	Initial concentration (mg/L)
Nitrate	7.00	71.17	74.84	28.29
Nitrite	7.97	78.48	65.72	28.44

VI. Application of the Optimized Adsorption Method to Real Samples

After determining the optimum parameters as shown in Table 2, the parameters were applied in a 50 mL of the wastewater sample and the resulting solution was analysed using IC. The percentage removal of ions was calculated using the formula below:

$$\frac{Ci-Cf}{Ci} \times 100 \quad (1)$$

Where; C_i is the initial concentration of metal ions in wastewater sample, C_f is the final concentration of nitrate and nitrite anions in wastewater after applying the VFSWR. The percentage removal of nitrate and nitrite were 91.42% and 74.60% with % RSD of 1.44% and 2.09% respectively after the experiment was done in triplicate as showed in Figure 4.

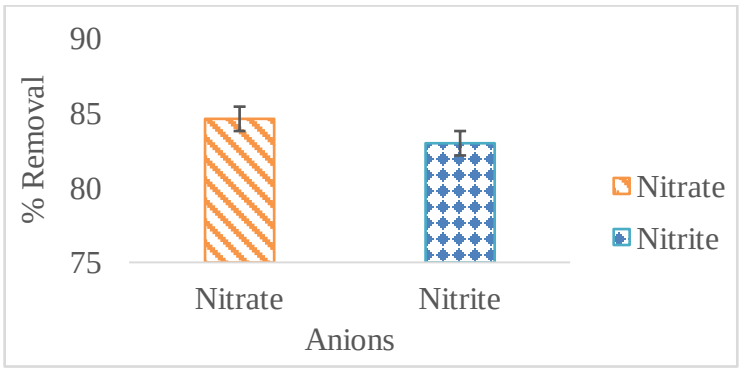

Figure 4: Percentage removal of nitrate and nitrite anions by VFSWR from wastewater

VII. Adsorption Kinetics

In order to define the adsorption kinetics of the anions, the kinetic parameters for the adsorption processes were studied for the VFSWR. The contact times employed for the experiment were ranging between 1 to 90 min and first order, second order and intra particle diffusion models were applied to the experimental data employing mathematical models. The first order kinetic equation is

$$\log(q_e - q) = \log(q_e) - \frac{k_1}{2.303} t \quad (2)$$

Where *qe* and *q* are the adsorption capacity at equilibrium and at time t respectively and k_1 is the rate constant of the pseudo first order adsorption process.

Plot of $\log(q_e\text{-}q)$ vs. t gives a straight line for first order adsorption kinetics and the rate constant k_1 is computed from the plot.

The sorption data was also studied by second order kinetics

$$\frac{t}{q} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e} \quad (3)$$

The applicability of this equation can be studied by a plot of t/q vs. t. Intra particle diffusion was observed using the relationship between specific sorption (q) and the square root of time ($t^{1/2}$). The relation is expressed as follows:

$$q = k_d t^{1/2} \quad (4)$$

The pseudo first order was not satisfactory to explain the experimental data, whereas the calculated, q_{cal} values derived from the pseudo second order model for sorption of the anions were very close to the experimental (q_{exp}) values. The second order equation appeared to be the better fitting model than first order and intra particle diffusion equations because it has higher R^2 value as shown in Table 3[11].

Table 3: Adsorption Kinetics parameters of the VFSWR

Anions	q_{exp} (mg/g)	Second Order			First Order			Intra Particle Diffusion	
		R^2	K_2 (gmg^{-1}min^{-1})	q_{cal} (mg/g)	R^2	K_1 (min^{-1})	q_{cal} (mg/g)	R^2	K_d (mgL^{-1}min$^{-1/2}$)
NO_2^-	12.47	0.9976	0.036	12.92	0.9278	0.022	0.15	0.6343	0.288
NO_3^-	12.10	0.9976	0.046	12.95	0.9297	0.022	0.15	0.5898	0.108

VIII. Thermodynamics Parameters

The changes in Gibbs free energy (ΔG), enthalpy (ΔH) and entropy (ΔS) for the adsorption process were obtained using the following equations

$$lnb = \frac{\Delta S}{R} - \frac{\Delta H}{RT} \quad (5)$$

$$\Delta G = \Delta H - T\Delta S \quad (6)$$

Where R (8.314 J/mol K) is the gas constant, T (K) the absolute temperature and b (L/mol) the thermodynamic equilibrium constant. As reflected by the R^2 values shown in Figure 5the plot of Gibbs free energy (ΔG) versus temperature for VFSWR was found to be linear.

The negative values for the Gibbs free energy for all the anions, show that the adsorption process is spontaneous and that the degree of spontaneity of the reaction increases with increasing temperature [12]. The overall adsorption process seems to be endothermic (ΔH =46.19 and 51.25 kJmol-1 for NO_2^- and NO_3^- respectively). The ΔS values were positive (which implies that entropy increases as a result of adsorption). This occurs as a result of redistribution of energy between the adsorbate (NO_2^- and NO_3^-) and adsorbent (VFSWR).

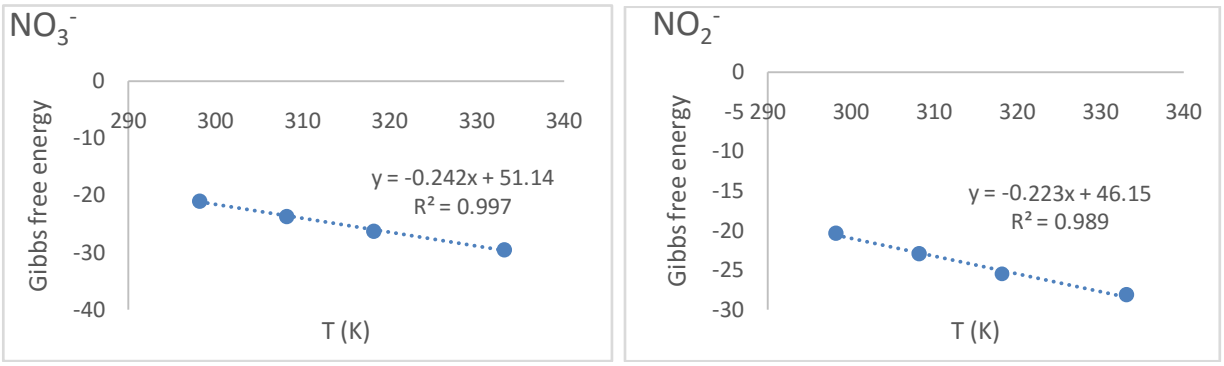

Figure 5: Adsorption thermodynamics of NO3- and NO2- by the VFSWR

IX. Conclusion

This study indicated that valuarized fish scales waste remains, which is widely available at no cost, can be used as an efficient adsorbent for removal of NO_2^-, and NO_3^- from wastewater. IR spectrum analysis suggested the different functional groups which are present in the given samples are OH, CH stretching, C=C stretching, C-O stretching. The thermodynamic study shows that the adsorption of the anions was of endothermic nature. The negative values of ΔG reveal the feasibility and spontaneity of the process. Initial concentration of adsorbates, pH, contact time, VFSWR dosage and adsorbent characteristics are the factors responsible for anions adsorption capability. This study demonstrated that valuarized fish scales waste remains are environmentally friendly, economical and readily available waste materials with high efficacy for the removal of excess toxic anions from wastewater as shown by the two model anions, NO_2^-, and NO_3^-.

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Effects of Mixed Rice Husk and Corn Cob as Fillers on Some Properties of Flexible Polyether Foam

By P.U. Chris-Okafor, R.U. Arinze, U.E. Ekpunobi & M.C. Anugwom
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Abstract- This work studied the effects of local fillers; rice husk and corn cob, on flexible polyether foam. These fillers were mixed in the ratio of 50:50. The foam samples were produced using polyol and other recipes for foam production in the appropriate formulations. Varying loads of the mixed fillers of particle size of 0.25mm, such as, 5%, 10%, 15%, 20% and 25% were incorporated into the foam. The physico-mechanical tests carried out on the foam samples were; density, hardness, compression, tensile strength and elongation at break. The creaming time, rising time, ignition time, char formation, char temperature and char duration of flexible polyether foam were also observed. The results showed that all the filled foams have higher densities than the unfilled foams as increase in filler loads increased the density of the foam samples. The fillers also modified other properties more than the unfilled foam used as a standard. The results of the flame tests showed that with increase in filler loads, the flammability of the produced foam was observed to be reduced. Hence, mixed rice husk and corn cob can be used as flame retardant in foam production and to improve other properties of the foam like density, load bearing ability and durability. More so, these fillers are agricultural wastes, completely organic and eco friendly, thus, can be used to produce biodegradable polyurethane foams.

Keywords: *rice husk, Corn cob, flexible polyether foam, mechanical and flammability properties.*

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I. Introduction

Polyurethane products are everywhere, it is found in every area of human activities. Flexible polyurethane foams are one of the most important classes of cellular plastics and can be applied in the fabrication of a wide range of materials for different uses such as foam mattresses, pillows, furniture, cushioning materials for automobiles, packing, recreation, shoes, [1]. The versatility of polyurethane chemistry permits the production of a great variety of materials such depending on the initial ingredients used in the synthesis [2]. Its usefulness has displaced rubber foam in these applications because of improved strength, lower density and easier fabrication.

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This in turn necessitated the incorporation of a variety of fillers into foam samples. Filler denotes any material that is added to polymer formulation to lower its cost or to improve its properties. The use of fillers to modify properties of composition can be dated back to at least middle of 19th Century in Roman era when artisans used ground marble, calcium carbonate ($CaCO_3$) in lime plaster, frescoes and pozzolanic mortar, paper and paper coating [3]. The higher the degree of the surface area of the filler, the higher it's stiffening ability on the polymer. Fillers can be classified in many different ways ranging from their shapes to specific characteristics: Extender fillers and functional fillers are classes based on performance [4].

In general, industries that produce flexible polyurethane foams use fillers to modify the material's properties in some way, such as: dimensional stability, retraction from the mold and density [5-6]. When adding filler to a polymer to form a conjugated biphasic material, the tension applied to the polymeric matrix will be transferred in part to the disperse phase, the filler, since it presents properties superior to the pure polymer [7]. Efficient reinforcement is achieved by interactions of the filler polymer matrix via mechanisms of adhesion, which could be: adsorption, electrostatic attraction, chemical bonding and mechanical adhesion [8]. Accordingly, it is necessary to know the end-use of the material in order to use the correct concentration in the polymer matrix, obtaining a product of reliable quality.

Many research works have been done on petrochemical based polyurethane systems using inorganic fillers like calcium trioxocarbonate (IV), talc, kaolin etc. But the quest for local, cheap, organic, readily available, bio-degradable and eco-friendly materials has spurned many researchers into finding materials that can used as fillers for polyurethane foams. Some of these researches include the use of agricultural materials especially wastes as fillers incorporated into polyurethane foams. And the effects of various agricultural and organic materials as fillers in flexible polyether foam have been studied, which include: effects of coconut husk and corn cob as fillers in flexible polyurethane foam [9], effects of mixed organic materials as filler on the physico-mechanical properties of flexible polyether foam [10], the effect of coconut and palm kernel shells on density, porosity index and tensile

properties of flexible polyether foam [11], palm kernel shell powder as filler in flexible polyether foam [12], etc. Chemicals used for the production of flexible polyether foam are: toluene diisocyanate, polyol, amine, stannous octoate, silicon oil and additives such as colourants, fillers, flame retardants, water and auxiliary blowing agents are also used [13]. Flexible polyether foams of different types have been produced using these chemicals. Such foams are used in various fields of life such as bedding, upholstery, laminated clothing and packaging. It also has good acoustic properties due to its structure [14].

Therefore, this study is to provide additional information on the effects of mixed rice husk and corn cob as fillers. These materials are locally available agro-wastes, lingo-cellulosic and relatively inexpensive as such that they can lower resin costs, improve stiffness and also can serve as eco-friendly materials to reduce the over dependence on petroleum-based plastics and reduce land-fills.

II. Materials and Methods

a) Samples collection and preparation

The polyurethane chemicals; polyol, toluene diisocyanate (TDI), silicone, stannous octoate, amine and water, used were sourced from Winco Foam Manufacturing Company in Awka, Anambra State. The local agricultural materials used as fillers; rice husk was sourced from Rice Mill in Abakaliki, Ebonyi State, while corn cob was sourced from Ifite, Awka, Anambra State both in Nigeria.

The rice husk and corn cob were washed with clean water to remove dust and unwanted impurities respectively. These were then dried under the sun for seven days, ground to fine powder and sieved by Gilson Automatic Sieve Tester, SS-15 model to pass through mesh sizes of 2mm, 1.6mm, 1.4mm, 0.8mm, 0.4mm and 0.25mm. The particle mesh size of 0.25mm was used for the two fillers to enhance easy homogeneity of the fillers.

b) Preparation of flexible polyether foam

125g of each of the fillers; rice husk and corn cob were weighed and mixed thoroughly to obtain a homogenous mixture containing 50% of each of the filler. 25g, 50g, 75g, 100g and 125g (5%, 10%, 15%, 20% and 25%) of the mixed fillers were weighed out respectively by using an electrical weighing balance of Model D-72336 Made in China. The percentage was based on the quantity of the polyol used. Polyol and toluene diisocyanate were weighed out and poured into separate mixing containers. Appropriate quantities of water, amine, silicone oil and glycerin were weighed separately using syringes for the purpose of an accurate stoichiometric reaction.

The measured silicon, water, amine and glycerin were poured into the beaker containing the polyol and mixed filler, this was stirred properly. Stannous octate was poured into the mixture and stirred for 10seconds. Then the measured toluene diisocyanate was poured into that same mixture and stirred. At this stage the creaming time was taken.

The mixture was transferred into mould with dimensions of 8 x 8x 8cm and the rising time (time taken to attain full height) was also taken with a stop watch. This process was repeated for the different weights of filler.

Ten minutes after full rise was attained, the foam samples were removed from the mould and allowed to cure for 24 hours before characterization. This was also repeated for the different foam samples based on their gram weight.

c) Foam Formulation

The choice of the weights of the raw materials to be used in foam production is not made arbitrarily, it is chosen on the basis of formulation (Biodun, 2000). If a high –density foam is desired, the tendency is that the volume of water used will be reduced; this is due to the fact that density is universally related to volume. Table 1 below showed the formulation of the produced foam samples.

Table 1: Foam Formulation

Material	Pphp	F_0	F_1	F_2	F_3	F_4	F_5
Polyol (g)	100	500	475	450	425	400	375
Filler (g)	0	0	25	50	75	100	125
TDI (g)	53	265	251.76	238.50	225.25	212	198.75
Silicone oil (mL)	0.90	4.50	4.28	4.05	3.83	3.60	3.38
Amine (mL)	0.20	1.00	0.95	0.90	0.85	0.80	0.75
Tin (mL)	0.15	0.75	0.71	0.68	0.64	0.60	0.56
Water (mL)	4.30	21.50	20.43	19.35	18.28	17.20	16.12
Glycerin (mL)	1.00	5.00	4.75	4.50	4.25	4.00	3.75

Note : pphp= parts per hundred of polyol

F_0, F_1, F_2, F_3, F_4 and F_5 = 0%, 5% (25g), 10% (50g), 15% (75g), 20% (100g) and 25% (125g) filler loads respectively.

d) Characterization of Foam Samples

The following mechanical properties of the foam samples were determined using standard methods: density [15], while tensile strength, elongation-at-break, compression strength and hardness test were measured according to the ASTM-D standard specifications [16]. Its flammability tests were analyzed via flame duration, ignition time and char formation.

III. Results and Discussion

The results of the physico-mechanical properties of the foam samples were observed. The particle size of the filler has a dominating effect on these mechanical properties. Fillers become increasingly reinforcing as their particle size decreases in order to enable a large surface area for the polymer matrix-filler interaction.

a) Results of the mechanical properties tests

Table 2: Readings for the density test

Filler Load (%)	Filler load(g)	Density(kg/m^3)
0	0	20.03
5	25	20.06
10	50	21.98
15	75	21.22
20	100	31.89
25	125	34.48

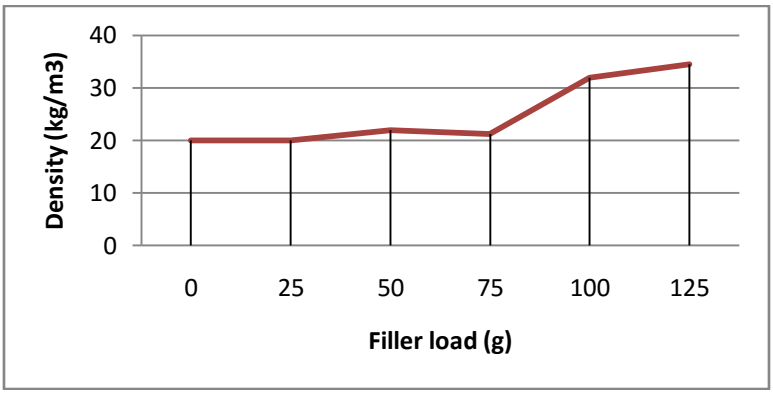

Fig. 1: Effect of filler load on density of the foam samples

From Table 2 and Fig.1, it is observed that increase in filler load causes increase in density of the foam samples. This could be attributed to the nature and high content of fillers which would fill up more voids, thus increasing its density. In flexible polyurethane foams, the fillers promote an increase in density and resistance to compression [14]. Density test helps to predict the performance of foam in their cushioning application as it predicts its durability and its ability to support and to push-back against weight and prevent foam collapse. This is in agreement with some other works [11, 12].

Table 3: Readings for the compression set test on the foam samples

Filler Load (%)	Filler Load(g)	Compression Set (%)
0	0	3.7
5	25	7.69
10	50	4.17
15	75	7.63
20	100	8.70
25	125	4.55

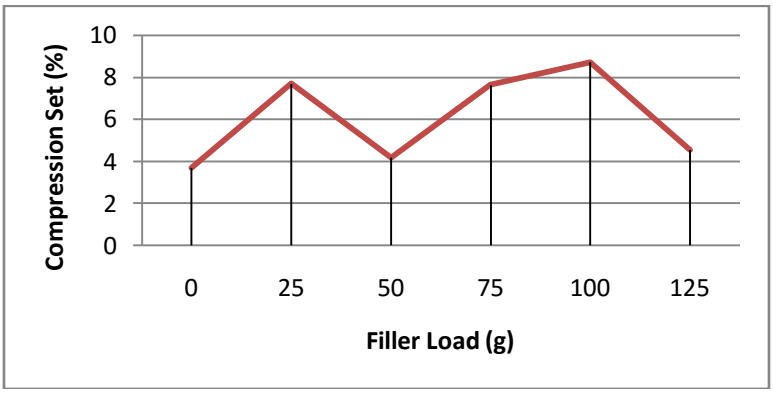

Fig. 2: Effect of filler load on compression set of the foam samples

It is observed that the fillers increased the compression strength of the foam, as shown in Table 3 and Fig. 2. Although, there was a varying trend in the decrease at filler loads of 50g and 125g respectively. This showed that the presence of filler improved the possibility of foam to return to its original size. This is one of the qualities of good and durable foams. It could be due to reinforcing property exhibited by the filler as a result of its cellulosic nature. From the result above, it is also observed that the decrease in compression strength at 125g filled foam, inferred that though125g filled foam sample has the highest density, still it has a low ability to return to original size after compression, hence it is evident that the density of a foam sample has no direct effect on its compression [13]. The increased compression set also agrees with the works of some other authors [10,11,12].

Table 4: Readings for the tensile strength test on the foam samples

Filler (%)	Filler load (g)	Tensile strength (MPa)
0	0	83.21
5	25	114.34
10	50	116.37
15	75	125.05
20	100	106.48
25	125	91

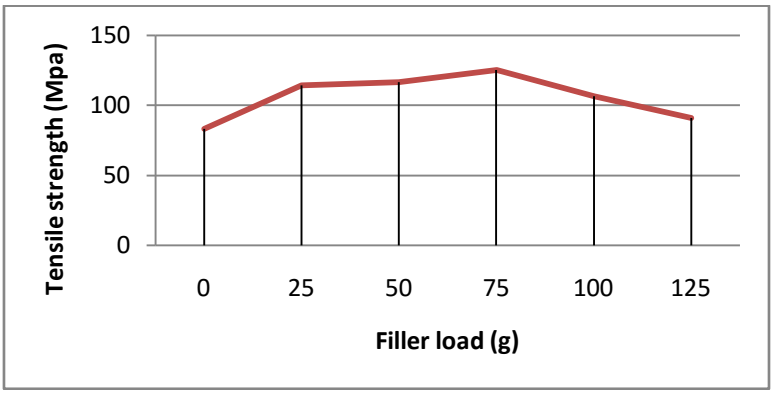

Fig. 3: Effect of filler load on tensile strength of the foam samples

It is observed that the tensile strength increased as the filler load increased as evident in Table 4 and Fig.3. This enhanced property could be attributed to good interaction between filler-polymer matrix. It could also be due to nature and small particle size of the filler thereby providing a good surface area to resist stress. Since, additives and fillers are added to improve the mechanical properties of foam [11,13].

Table 5: Readings for % Elongation

Filler (%)	Filler Load (g)	% Elongation
0	0	130.10
5	25	128.23
10	50	116.37
15	75	109.12
20	100	106.48
25	125	94.43

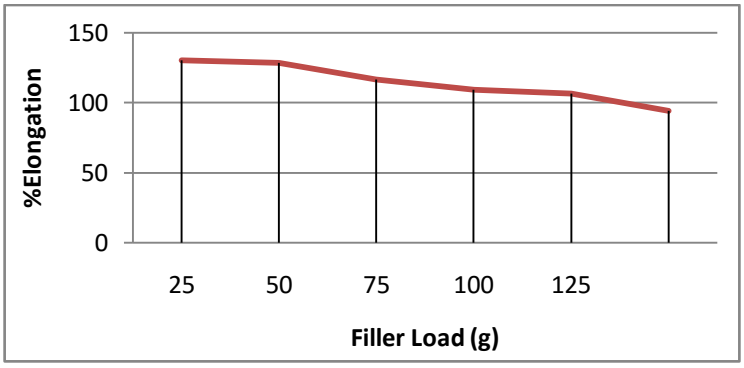

Fig. 4: Effect of filler load of %elongation of the foam sample

It is evident that the fillers decreased the % elongation-at-break of the foam samples as seen in Table 6 and Fig. 4 above. The cellulosic nature of the filler could be attributed to this effect that led to its tendency to elongate with a lesser filler ratio than a higher one. This also agrees with other works [10, 13].

Table 6: Readings for indentation force deflection (IFD) or hardness test

Filler Load (%)	Filler Load(g)	25%	40%	65%
0	0	28.3	38.0	71.5
5	25	32.0	40.6	84.3
10	50	43.2	52.6	101.5
15	75	47.4	61.4	109.8
20	100	35.9	46.6	91.1
25	125	58.8	69.9	123.5

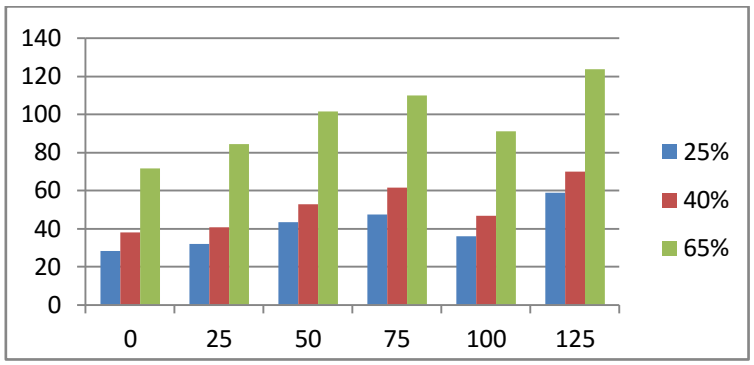

Fig. 5: Effect of filler load on IFD of the foam sample

It is evident that the hardness of the produced foam increased as filler load increased. This is as shown in Table 6 and Fig.5. The 65% IFD exhibited the highest hardness and this could be due to the nature and particle size of the fillers as well as the interactions between the polymer matrix-filler phase. 25% and 40% showed values less than 65% though the increase in hardness was displayed. The filler added in foam formulation modify the foam's hardness, improving the dimensional stability. Hence the increase in filler load increases the load bearing properties of the foam sample. This also agrees with the works of some other authors [11, 17].

Table 7: Readings of creaming, rising and curing time

Filler Load (%)	Filler Load(g)	Cream time (sec)	Risingtime (sec)	Curing time(hr)
0	0	13	30	24
5	25	15	28	24
10	50	16	24	24
15	75	10	20	24
20	100	18	17	24
25	125	22	11	24

From Table 7 above, the creaming time of the foam samples increased as the filler load is increased. This shows that as the filler load is increasing, the creaming time is been delayed. Delay in creaming time is often essential for the production of complex parts particularly for multiple hardness foam cushions. Also, the variation in the rising time of the foam samples showed a uniform decrement in rise time as the filler load increases. This implies that the foam rises faster when the filler composition increases indicating that the blowing / gas production reaction between toluene diisocyanate and water occurs faster. It could therefore be deduced that the introduction of fillers in foam formulation greatly influences the reaction time which is a positive development; while the curing time was observed to be constant for all the filled samples.

Table 8: Readings of flammability test of the foam samples

Filler Load (%)	Filler Load(g)	Ignition Time(sec)	Flame Duration(sec)	Char Formation(sec)	Char Temp(^{0}C)
0	0	2	196	2	49
5	25	3	161	3	53
10	50	5	162	5	61
15	75	3	165	3	69
20	100	6	147	6	62
25	125	8	88	8	58

The ignition time was observed to increase as filler load increased as seen in Table 8 above. This implies that increase in filler load increases the ignition time of the foam samples and this is the same for the char formation except for 15% foam which has the same time as the 5% foam sample. The flame duration decreased as filler load increased. This shows that the presence of filler reduces the flame duration. Thus, this entails that mixed rice husk and corn cob can be used as a flame retardant in foam production.

IV. Conclusion

The results of the effects of the mixed filler; rice husk and corn cob on the flexible polyether foam samples showed the reinforcing abilities of the fillers. This could be attributed to the small mesh size of the mixed filler; that created a good surface area for the filler- polymer matrix interaction thereby enhancing the foam's mechanical properties. The filler also exhibited the tendency of flame reduction and can be used since polyurethane foams are highly inflammable.

The research showed that at 75g-100g concentrations of the filler gave the best reinforcing properties. Thus, moderate incorporation of filler can be used to give desired quality of products. Density of a foam sample has no direct effect on its creaming time, rising time and compression set. The load bearing properties of foam increases with increase in filler load. Good quality and flame retarding foam can be cheaply produced using easily accessible fillers like rice husk and corn cobs.

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Note :

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4. Manuscript's Category,

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1. Choosing the topic: In most cases, the topic is searched by the interest of author but it can be also suggested by the guides. You can have several topics and then you can judge that in which topic or subject you are finding yourself most comfortable. This can be done by asking several questions to yourself, like Will I be able to carry our search in this area? Will I find all necessary recourses to accomplish the search? Will I be able to find all information in this field area? If the answer of these types of questions will be "Yes" then you can choose that topic. In most of the cases, you may have to conduct the surveys and have to visit several places because this field is related to Computer Science and Information Technology. Also, you may have to do a lot of work to find all rise and falls regarding the various data of that subject. Sometimes, detailed information plays a vital role, instead of short information.

2. Evaluators are human: First thing to remember that evaluators are also human being. They are not only meant for rejecting a paper. They are here to evaluate your paper. So, present your Best.

3. Think Like Evaluators: If you are in a confusion or getting demotivated that your paper will be accepted by evaluators or not, then think and try to evaluate your paper like an Evaluator. Try to understand that what an evaluator wants in your research paper and automatically you will have your answer.

4. Make blueprints of paper: The outline is the plan or framework that will help you to arrange your thoughts. It will make your paper logical. But remember that all points of your outline must be related to the topic you have chosen.

5. Ask your Guides: If you are having any difficulty in your research, then do not hesitate to share your difficulty to your guide (if you have any). They will surely help you out and resolve your doubts. If you can't clarify what exactly you require for your work then ask the supervisor to help you with the alternative. He might also provide you the list of essential readings.

6. Use of computer is recommended: As you are doing research in the field of Computer Science, then this point is quite obvious.

7. Use right software: Always use good quality software packages. If you are not capable to judge good software then you can lose quality of your paper unknowingly. There are various software programs available to help you, which you can get through Internet.

8. Use the Internet for help: An excellent start for your paper can be by using the Google. It is an excellent search engine, where you can have your doubts resolved. You may also read some answers for the frequent question how to write my research paper or find model research paper. From the internet library you can download books. If you have all required books make important reading selecting and analyzing the specified information. Then put together research paper sketch out.

9. Use and get big pictures: Always use encyclopedias, Wikipedia to get pictures so that you can go into the depth.

10. Bookmarks are useful: When you read any book or magazine, you generally use bookmarks, right! It is a good habit, which helps to not to lose your continuity. You should always use bookmarks while searching on Internet also, which will make your search easier.

11. Revise what you wrote: When you write anything, always read it, summarize it and then finalize it.

12. Make all efforts: Make all efforts to mention what you are going to write in your paper. That means always have a good start. Try to mention everything in introduction, that what is the need of a particular research paper. Polish your work by good skill of writing and always give an evaluator, what he wants.

13. Have backups: When you are going to do any important thing like making research paper, you should always have backup copies of it either in your computer or in paper. This will help you to not to lose any of your important.

14. Produce good diagrams of your own: Always try to include good charts or diagrams in your paper to improve quality. Using several and unnecessary diagrams will degrade the quality of your paper by creating "hotchpotch." So always, try to make and include those diagrams, which are made by your own to improve readability and understandability of your paper.

15. Use of direct quotes: When you do research relevant to literature, history or current affairs then use of quotes become essential but if study is relevant to science then use of quotes is not preferable.

16. Use proper verb tense: Use proper verb tenses in your paper. Use past tense, to present those events that happened. Use present tense to indicate events that are going on. Use future tense to indicate future happening events. Use of improper and wrong tenses will confuse the evaluator. Avoid the sentences that are incomplete.

17. Never use online paper: If you are getting any paper on Internet, then never use it as your research paper because it might be possible that evaluator has already seen it or maybe it is outdated version.

18. Pick a good study spot: To do your research studies always try to pick a spot, which is quiet. Every spot is not for studies. Spot that suits you choose it and proceed further.

19. Know what you know: Always try to know, what you know by making objectives. Else, you will be confused and cannot achieve your target.

20. Use good quality grammar: Always use a good quality grammar and use words that will throw positive impact on evaluator. Use of good quality grammar does not mean to use tough words, that for each word the evaluator has to go through dictionary. Do not start sentence with a conjunction. Do not fragment sentences. Eliminate one-word sentences. Ignore passive voice. Do not ever use a big word when a diminutive one would suffice. Verbs have to be in agreement with their subjects. Prepositions are not expressions to finish sentences with. It is incorrect to ever divide an infinitive. Avoid clichés like the disease. Also, always shun irritating alliteration. Use language that is simple and straight forward. put together a neat summary.

21. Arrangement of information: Each section of the main body should start with an opening sentence and there should be a changeover at the end of the section. Give only valid and powerful arguments to your topic. You may also maintain your arguments with records.

22. Never start in last minute: Always start at right time and give enough time to research work. Leaving everything to the last minute will degrade your paper and spoil your work.

23. Multitasking in research is not good: Doing several things at the same time proves bad habit in case of research activity. Research is an area, where everything has a particular time slot. Divide your research work in parts and do particular part in particular time slot.

24. Never copy others' work: Never copy others' work and give it your name because if evaluator has seen it anywhere you will be in trouble.

25. Take proper rest and food: No matter how many hours you spend for your research activity, if you are not taking care of your health then all your efforts will be in vain. For a quality research, study is must, and this can be done by taking proper rest and food.

26. Go for seminars: Attend seminars if the topic is relevant to your research area. Utilize all your resources.

27. Refresh your mind after intervals: Try to give rest to your mind by listening to soft music or by sleeping in intervals. This will also improve your memory.

28. Make colleagues: Always try to make colleagues. No matter how sharper or intelligent you are, if you make colleagues you can have several ideas, which will be helpful for your research.

29. Think technically: Always think technically. If anything happens, then search its reasons, its benefits, and demerits.

30. Think and then print: When you will go to print your paper, notice that tables are not be split, headings are not detached from their descriptions, and page sequence is maintained.

31. Adding unnecessary information: Do not add unnecessary information, like, I have used MS Excel to draw graph. Do not add irrelevant and inappropriate material. These all will create superfluous. Foreign terminology and phrases are not apropos. One should NEVER take a broad view. Analogy in script is like feathers on a snake. Not at all use a large word when a very small one would be sufficient. Use words properly, regardless of how others use them. Remove quotations. Puns are for kids, not grunt readers. Amplification is a billion times of inferior quality than sarcasm.

32. Never oversimplify everything: To add material in your research paper, never go for oversimplification. This will definitely irritate the evaluator. Be more or less specific. Also too, by no means, ever use rhythmic redundancies. Contractions aren't essential and shouldn't be there used. Comparisons are as terrible as clichés. Give up ampersands and abbreviations, and so on. Remove commas, that are, not necessary. Parenthetical words however should be together with this in commas. Understatement is all the time the complete best way to put onward earth-shaking thoughts. Give a detailed literary review.

33. Report concluded results: Use concluded results. From raw data, filter the results and then conclude your studies based on measurements and observations taken. Significant figures and appropriate number of decimal places should be used. Parenthetical remarks are prohibitive. Proofread carefully at final stage. In the end give outline to your arguments. Spot out perspectives of further study of this subject. Justify your conclusion by at the bottom of them with sufficient justifications and examples.

34. After conclusion: Once you have concluded your research, the next most important step is to present your findings. Presentation is extremely important as it is the definite medium though which your research is going to be in print to the rest of the crowd. Care should be taken to categorize your thoughts well and present them in a logical and neat manner. A good quality research paper format is essential because it serves to highlight your research paper and bring to light all necessary aspects in your research.

Informal Guidelines of Research Paper Writing

Key points to remember:

- Submit all work in its final form.
- Write your paper in the form, which is presented in the guidelines using the template.
- Please note the criterion for grading the final paper by peer-reviewers.

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 definite statistics - 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.
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- 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.

Please carefully note down following rules and regulation before submitting your Research Paper to Global Journals Inc. (US):

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- To guard yourself and others from possible illegal use please do not permit anyone right to use to your paper and files.

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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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