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## Chemistry

Frontier Chemistry Aspects

Dehydrogenation of Cyclohexanone

Highlights

Research of New Compounds

Chemopreventive Action of Compounds

**Discovering Thoughts, Inventing Future**

VOLUME 20 ISSUE 2 VRSION 1.0

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Chemistry

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# Frontier Chemistry Aspects

By Ordin S. V.
*Ioffe Institute RAS*

*Abstract-* Chemistry laid the foundations for a wide range of branches of science from physics to biology. Moreover, its basic algorithm, the chemical formula, can be said to underlie the construction of mathematical graphs and the quantum-mechanical description with their help (Richard Feynman) of the interaction of elementary particles. And Chemistry itself received a scientific justification from these sections of Physics. But when analyzing the NANO-scale missed by physics, it became clear that these justifications, which became dogmatic postulates, brought not only Physics itself, but also Chemistry to saturation in the approximation to the Truth. It was this saturation that led to various so-called anomalies. which, in fact, are simply going beyond the applicability of the models used. It primarily refers to the "understanding" of chemical bonds - in fact, to the canonization of orbitals calculated based on the Schrödinger equation. But as was shown earlier, the Schrödinger equation itself describes not the ELEMENTARY case but the PRIMITIVE. i.e. non-invariant for all chemical elements. Therefore, confining himself to Pauling's ersatz representations (which he abandoned later, but which were canonized) is a dead-end in the chemical construction of new materials.

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## I. Introduction

A lot of time has passed from the general definition of Chemistry by Lomonosov as the Science of Mixing-alloy (metals) and Separation. And during this time, there has been a significant detailing of the mixing / separation processes in liquid, gaseous, and even in solid solutions. And the general patterns of “mixing / separation” were found and fairly strictly described in both equilibrium and nonequilibrium processes. In initially within the framework of equilibrium thermodynamics, which stood out as an independent section of science. And then in nonequilibrium thermodynamics, which has become a continuation of the section that has arisen, which is more correctly called thermostatics, as involved in the calculations of thermodynamic equilibrium. Then, even in stationary flows, the appearance of both concentration solitons [1] and dissipative structures in the energy flow of the chemist Prigozhin [2] is possible. So, to describe the mixing/separation processes, a set of specific invariants has been formed, both spatial and temporal. These invariants, in their peculiar chemical way, reflected the essence / quintessence of understanding of Nature, which was basically implied by the word Chemistry. But, at the same time, the detailing and expansion of Chemistry went not only in the functional plan described above but also in the direction of determining MIXING ELEMENTS. This road was not always broad and straight - there were fantasies, like the same particles of phlogiston. Although their analysis was not at all useless and, one might say, formed the basis of that part of thermodynamics, which later migrated to physics. But the reincarnation of ancient Greek ideas about atoms was supplemented by a fundamentally new invariant molecule, the formula of which became the major "mathematical" tool, which distinguished Chemistry from the theories generated by it, which became sections of physics. The systematization of atoms by the periodic table and the introduction of the concept of chemical bonds made it possible to describe almost all of the observed substances. It was the FAITH in the Chemical Formula that even allowed the creation of boron nitride, non-existent on Earth, created in laboratory work by a 3rd-year student of the Leningrad Technological Institute B.N. Sharupin [3].

But this Faith in the Chemical Formula was already perceived as Scientific Truth due to extensive and precise physical research, and atoms, and molecules, and clusters, and single crystals. Even a macroscopic single crystal, say silicon, can be defined by the elementary chemical formula $Si_n$. More precisely, by the formula $Si_k)_n$, where k is the number of atoms in the formula in the unit cell. So it was the chemical approach that determined the relationship of quantum-mechanical calculations [4, 5] with the macroscopic properties of materials [6]. Conversely, physical investigation of dynamics, primarily the vibrations of atoms and electrons in various substances, made it possible to realize why and how atoms form molecules, i.e. understand the chemical bonds themselves, leading to the formation of the studied substances [7, 8,9].

### a) *Classical and quantum physical characteristics of chemical bonds*

One can say even in ancient Greek ideas about atoms in an implicit plan there are the Principle of Logarithmic Relativity [10] for spatial scales - tangible and observable “particles” -stones were projected onto the unobservable (previously) microworld of sandals worn to the invisibility of stones. Moreover, the behavior of microparticles was described like macroscopic description, but with a scale factor. And the scale factor was also borrowed from available limiting observations. Say, the difference in the relative thickness of the legs of an ant and an elephant is determined by the dependence of volume/mass on the cube of size

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obtained in macroscopy. In this regard, even purely classical atomic models in the form of balls, and the representation of chemical bonds by springs, allow us to describe lattice vibrations of crystals (Fig. 1) in the framework of an elementary? harmonic oscillator [11, 12] and, thus, say about hardness and strength crystal, about its heat capacity and heat resistance. In the end, and the rigidity and strength of the chemical bond itself. So, the "spring" stiffness used in the oscillator model determines the frequency of the transverse phonon $\omega_T$, which strictly corresponds, as shown in Fig. 1. for model reflection (pink curve enveloping the experimental reflection spectrum for cubic boron nitride), in simple crystals, to the low-frequency edge of the peak of lattice reflection.

An insignificant quantitative difference between the dome of the model spectrum of the lattice reflection (thin pink line) and the experimental spectrum of cubic nitride is associated with a small concentration of defects in the sample obtained by the explosion method from the rhombohedral modification. Whereas for the initial perfect sample of rhombohedral boron nitride and silicon carbide, the reflection spectra shown in Fig. 1 coincide with the experimental accuracy with the model spectra.

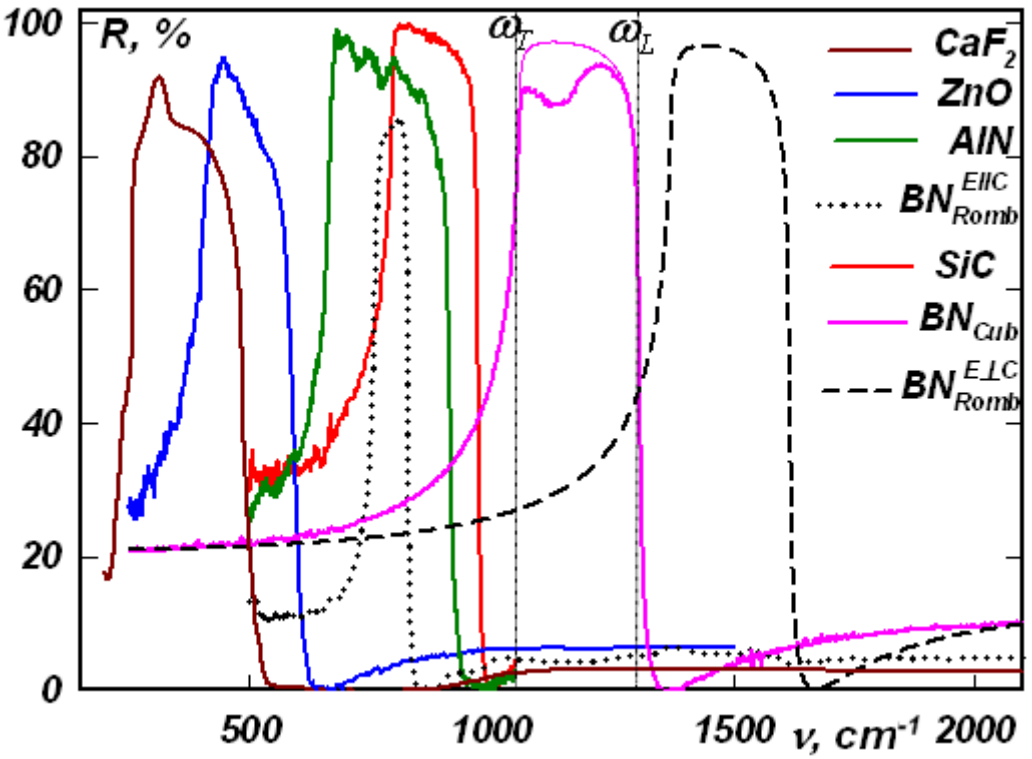


*Fig. 1:* Lattice reflection spectra of single crystals

But all the lattice reflection spectra of crystals with a simple unit cell are shown with high accuracy to determine which is determined $\omega_T$ by the rigidity of chemical bonds - springs and the reduced mass of atom balls.

So, this alone is enough to understand a lot. In particular, for isotropic crystals, their rigidity, which is of the utmost importance as in diamond, is an analog of cubic boron nitride. On the other hand, as can be seen from the figure, the stiffness of chemical bonds inside the atomic layers of hexagons is higher than the stiffness of bonds in a cubic modification. Also it can be seen from the figure that the interlayer interaction in rhombohedral boron nitride and in its conducting analog of graphite is determined by a small concentration of very hard chemical bonds [13, 14]. Their stiffness is approximately equal to the stiffness of bonds in silicon carbide, which is several orders of magnitude tougher than the van der Waals interaction, which is often used to describe the two-dimensionality of some crystals [15] (which directly contradicts their high heat resistance).

Moreover, as specially carried out studies of the size effect in the lattice absorption of silicon carbide have shown [ 16, 17, 18], the dipole vibration frequency in monotonously lay samples varies from the transverse frequency in a SiC single crystal to the vibration frequency in a molecule in a polycarbosilane molecule (Fig. 2).

The high-frequency edge of the grating reflection peaks is determined by the so-called plasma addition $\omega_P$ due to the charge of the Sighetti dipole — the shift of the electron density towards one of the

atoms of the chemical unit cell formula and the concentration of dipoles in the crystal lattice. This plasma addition to the transverse frequency determines the frequency of the longitudinal phonon $\omega_L$, which determines the high-frequency edge of the lattice reflection

$$\omega_L^2 = \omega_T^2 + \omega_P^2 \quad (1)$$

The frequency of the longitudinal phonon $\omega_L$ directly characterizes the tensile strength of the chemical bond — the maximum energy of its breaking and, thereby, the strength of the material and its melting temperature. A plasma additive is directly related to the strength of the oscillator in the single-oscillator model used for simple crystals.

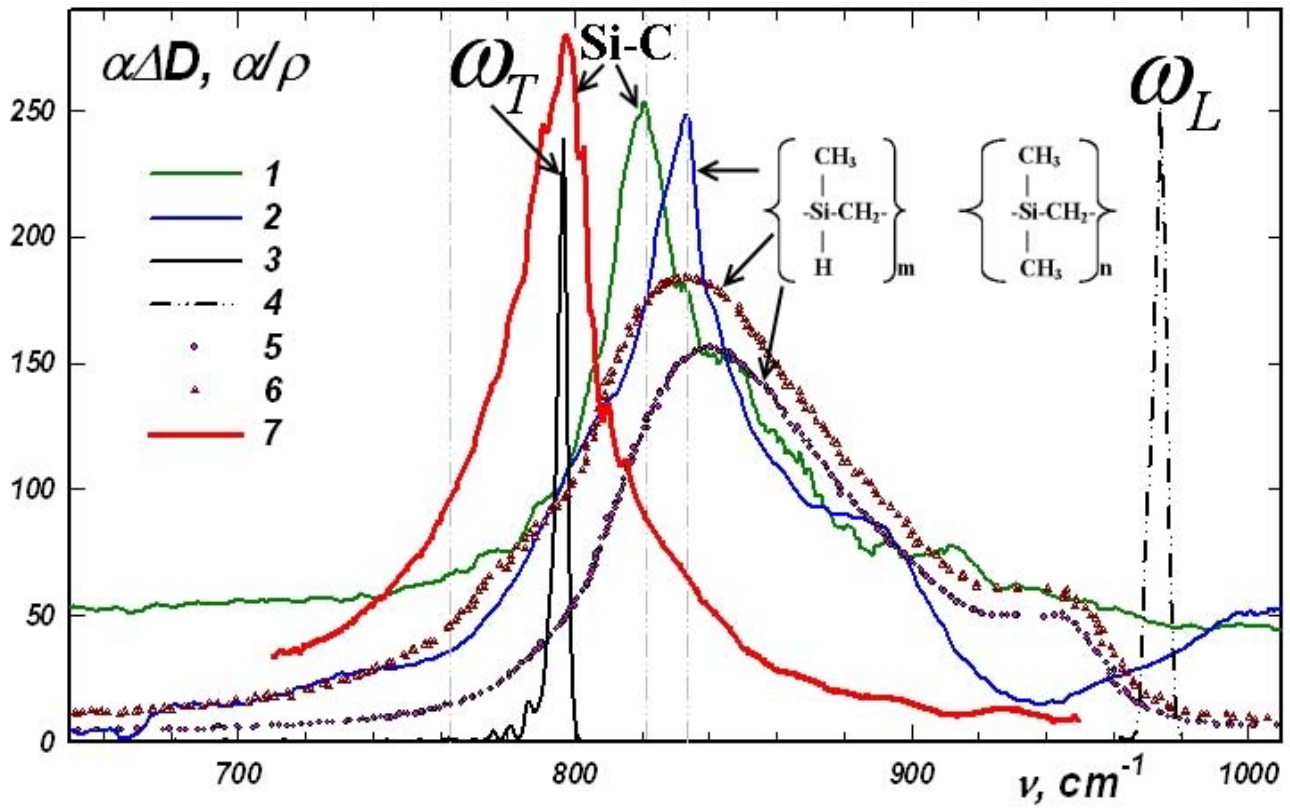


*Fig. 2:* Absorption spectra of Si-C dipoles in different samples: 1-micron powder of silicon carbide, 2 – SiC molecule in polycarbosilane, 3 and 4 - $\omega_T$ and $\omega_L$ , accordingly, from the reflection spectra of a silicon carbide single crystal, 5 and 6 - SiC nanoparticles in annealed polycarbosilane, 7 - absorption of single-crystal silicon carbide films

The single-oscillator model of lattice reflection can be described for most crystals. But the absorption maxima shown in Fig. 2 corresponds only to electro-active vibrations, whereas, as is well known in materials, there is a rich set of atomic vibrations from zero frequency to $\omega_L$. Not all vibrational levels are IR-active - have an impulse not equal to the impulse of light used for the diagnosis of infrared radiation. But all of them are transformed from individual resonances into zones of allowed wave oscillations. Based on a single-oscillator model, all these wave oscillations can be qualitatively calculated in the form of phonon spectra $\omega(k)$:

$$\omega_{\pm}^2(k) = \frac{\xi}{M^*}\left(1 \pm \sqrt{1 - \frac{4M^*}{M_1 + M_2} Sin^2\left(k\frac{a}{2}\right)}\right) \quad (2)$$

Where $\xi$ - ion bond stiffness, $M_1$ и $M_2$ - ion masses, $M^* = \frac{M_1 M_2}{M_1 + M_2}$ - reduced mass of ions. Expressions for the phonon frequencies at the boundary of the Brillouin zone: $\omega_+(0) = \omega_T = \sqrt{\frac{2\xi}{M^*}}$ ,

$$\omega_+(a) = \sqrt{\frac{2\xi}{M_1}}, \omega_-(a) = \sqrt{\frac{2\xi}{M_2}} \quad (3)$$

The branches of transverse optical and acoustic phonons calculated using this formula, taking into account the corresponding SiC parameters, are presented in Fig. 3.

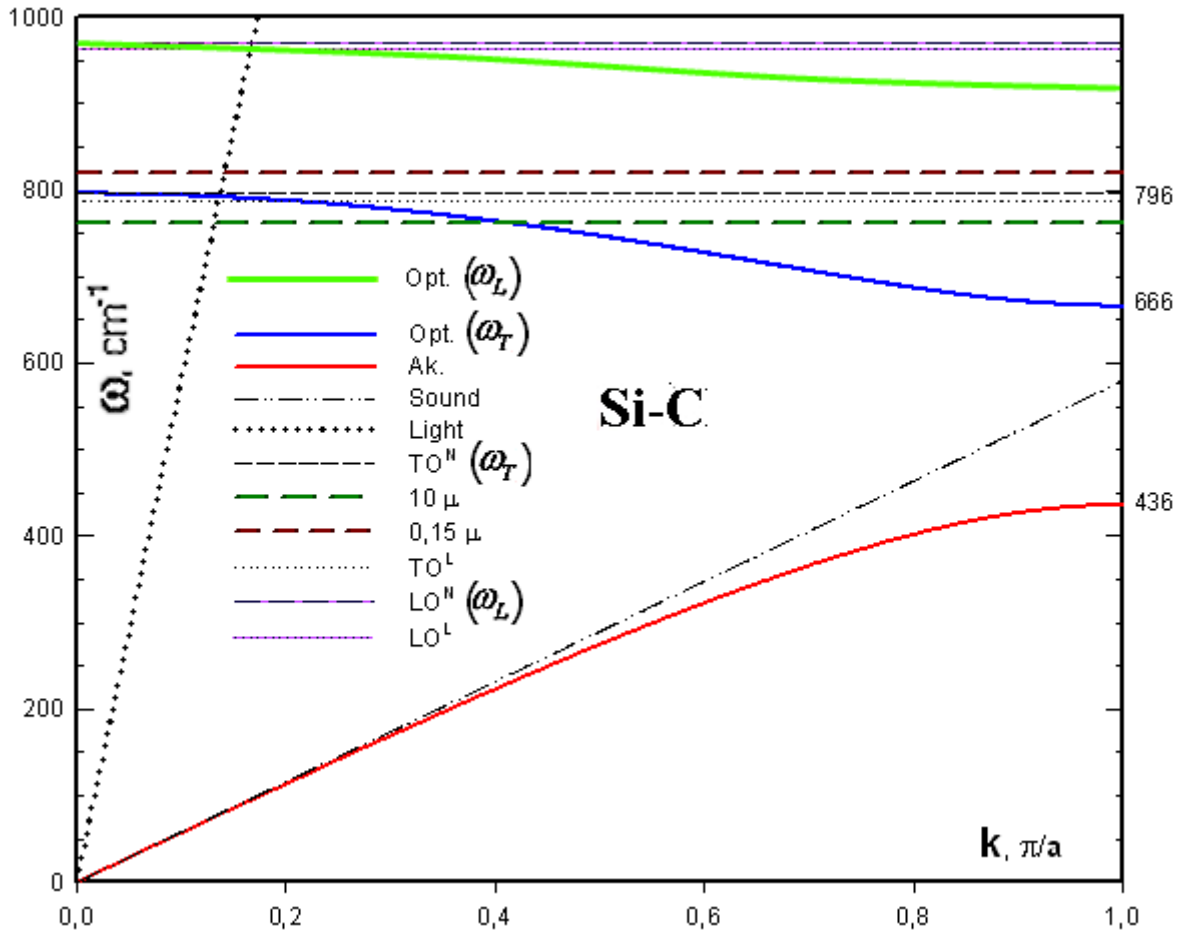


*Fig. 3:* Branches of transverse optical and acoustic phonons calculated by the above formula, taking into account the corresponding parameters of SiC

The highest line corresponds to the frequency of the longitudinal optical phonon

$$\omega_L = \sqrt{\omega_T^2 + \omega_P^*} \quad (4)$$

The slope of the lower asymptotics (dash-dotted line) determines the speed of sound$V_S$:

$$\omega_S = V_S k \quad (5)$$

The interaction of light with a lattice demonstrates the intersection of the law of dispersion of light (dashed line):

$$\omega = \frac{ck}{\sqrt{\varepsilon_\infty}} \quad (6)$$

with the branch of transverse phonons (blue line).

Figure 3 shows the frequency range of the allowed transverse vibrations in SiC. The asymptotics for sound (dash-dotted line) and the conditional dependence for light intersecting with the branch of transverse optical phonons are also shown. The dashed horizontal lines show the frequencies TO and LO at E perpendicular to the C axis, and dots at E parallel to the C axis for the 6H-SiC crystal. These lines show the maximum frequency range observed on single crystals.

The above analysis (possibly somewhat redundant for chemists) simply demonstrates that RESOLVED ENERGETIC ZONES (frequency bands are thick colored lines) ARE TRANSFORMED (due to the interaction of individual frequency levels) RESONANT LEVELS (Fig. 4). And, as shown in the book [8], the calculations of phonon spectra based on a quantum oscillator violate this causal relationship.

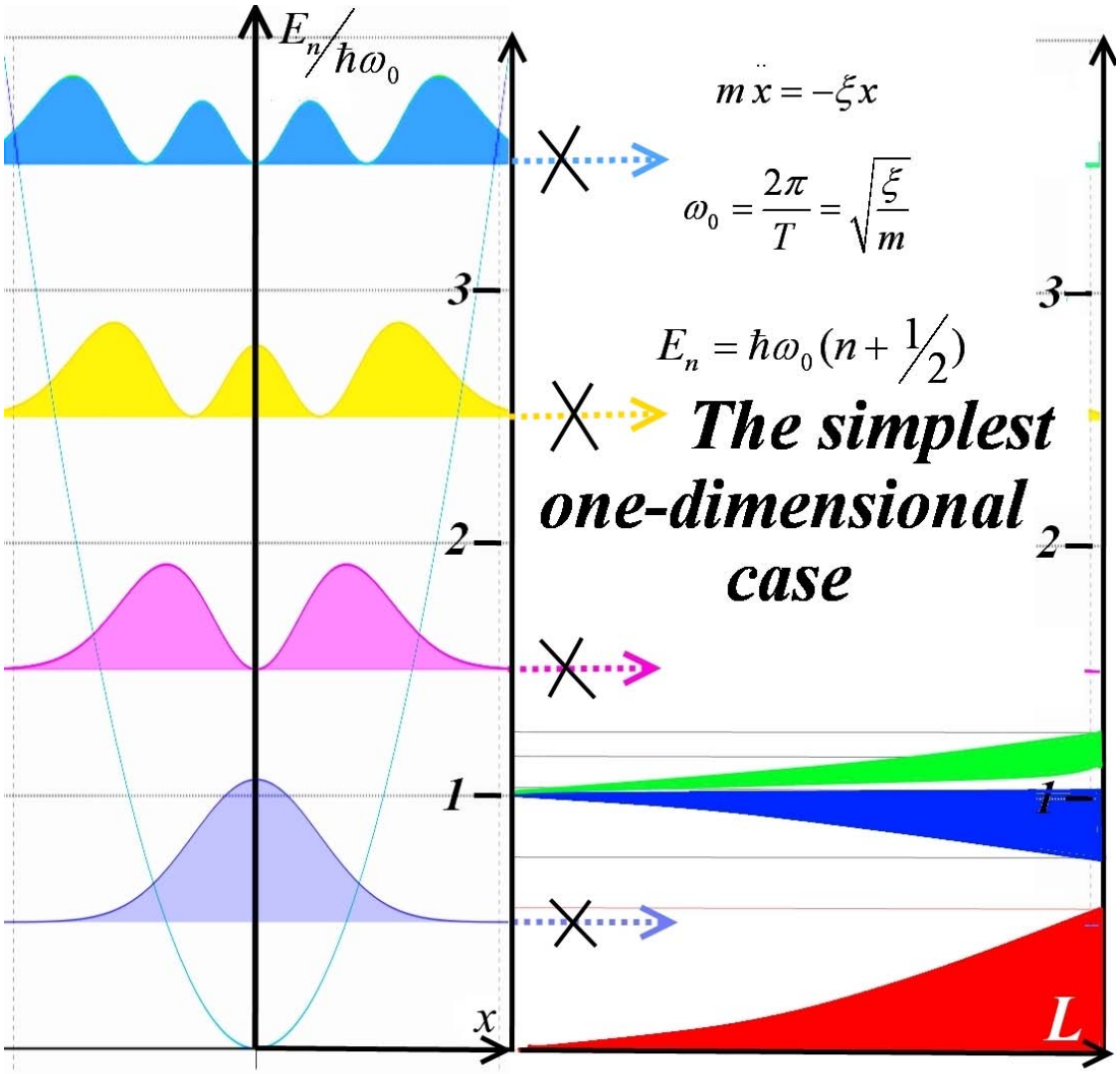


*Fig. 4:* Transformation of the levels of the classical harmonic oscillator into the allowed zones of the observed polaritons and acoustic waves (the color of the zones corresponds to Fig. 3 with an increase in the linear size of crystal *L*

The parabolic potential which is well shown in Fig. 4 gives a purely harmonic oscillation of a classical linear oscillator at a frequency $\omega_0$ (and 0) with the possibility of a continuous change in its oscillation amplitude *A* and its energy:

$$E = \frac{\xi A^2}{2} = \frac{m\omega_0^2 A^2}{2} \qquad (7)$$

But when rewriting the equations for the classical oscillator in the operator (Schroedger) form, second quantization is obtained, in which only spasmodic energy transitions between the energy levels shown in Fig. 4 are possible. At the same time, they received the first allowed level, which was attributed to unobservable ZERO vibrations. Whereas the transformation of the classical (first) level of vibrations into the zones of allowed energy states (Fig. 3) shown in Fig. 4 with an increase in the size of the (linear) particle *L* from an individual dipole to a single crystal corresponds to polaritons observed in lattice reflection and absorption (Fig. 1 and 2). Also, not mystical, but normal zero-point vibrations and they are also well studied in crystals, acoustic waves determine the lower allowed zone. Discrepancies in the fundamentals of second quantization indicated that in the case of operator overwriting even elementary equations, inaccuracy / non-rigor was allowed. But we will consider this contradiction in more detail in the analysis of atomic orbitals themselves, based on of which covalent or ion-covalent orbital-chemical bonds are formed.

For crystals having a complex unit (translatable) cell containing more than one dipole, instead of a continuous IR grating reflection band, we have, as shown in the example of quartz in Fig. 5, a whole set of oscillators associated with various atomic vibrations in the crystal lattice.

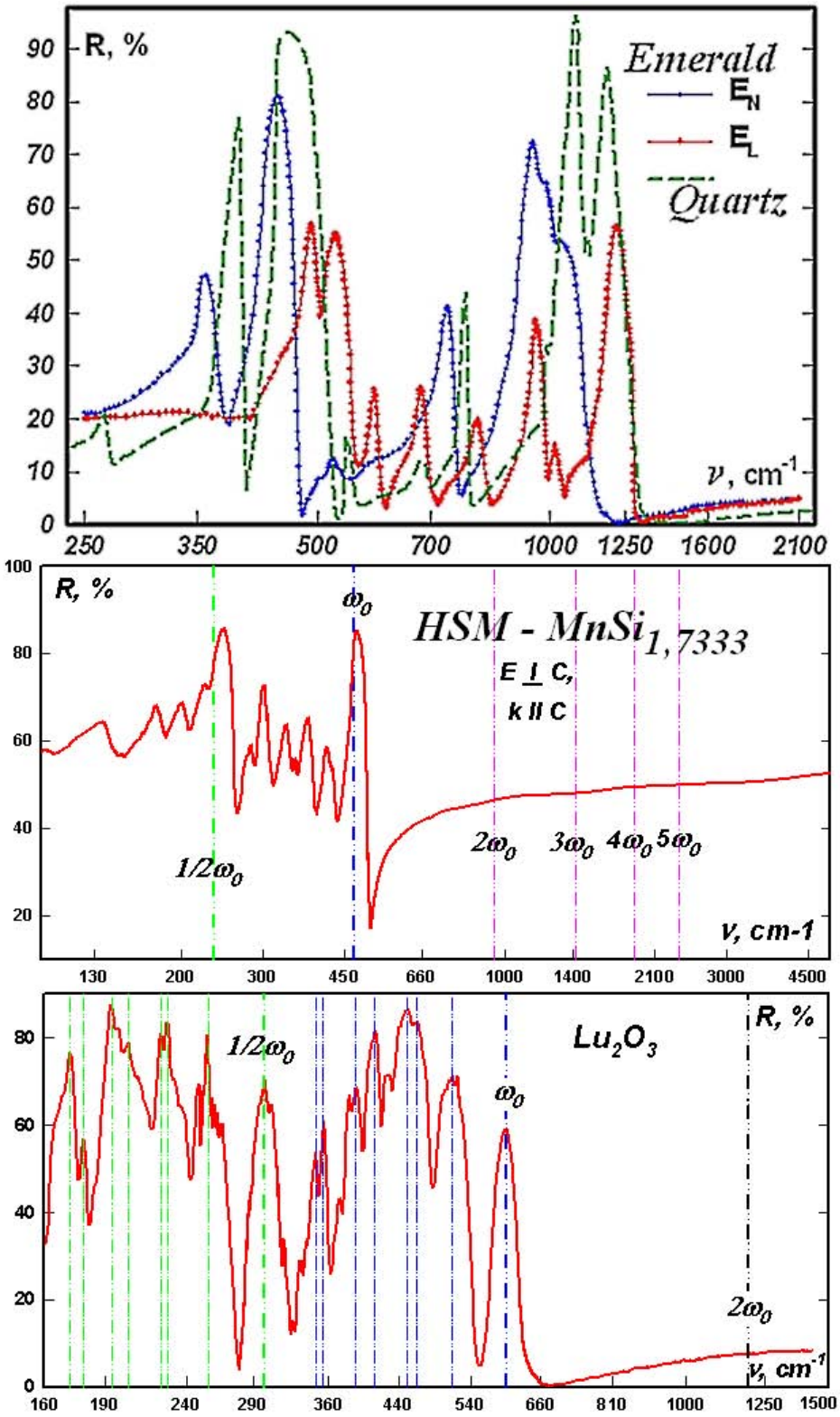


*Fig. 5:* Lattice reflection spectra of crystals with a complex unit cell.

And this complex set of oscillators observed in Fig. 5 is also described classically but by multi-oscillator models. And they even get correlations of physical properties with the calculated sum of the forces of all individual oscillators. But they are trying to describe formally and with the assumption that all oscillators are on the "spring" - known chemical bonds. Whereas from the subsequent consideration, it follows that the existence of previously unreported bonds due to new electronic orbitals is possible.

So the theory of phonons built based on of precisely the classical harmonic oscillator gave good agreement with experimental measurements and a lot of additional information about the properties of solids.

But the formal quantum-mechanical recalculation of the harmonic oscillator gave a set of frequencies (Fig. 4) that was not connected in any way with phonon branches. Whereas the formal quantum-mechanical recalculation of the harmonic oscillator yielded a set of frequencies (Fig. 4) that was not connected in any way with phonon branches. And the discrepancy between experiments with the prediction of the phonon theory is quite well eliminated, if, again, based on a clear classical model, we take into account the "springs" connecting the electron clouds with the atomic nucleus and the accompanying anharmonisms that violate the adiabatic decomposition into phonon and electron frequencies [8]. Moreover, it is likely that the quantum calculation of the first vibrational level violated the Heisenberg uncertainty principle.

Logically, physical chemistry must begin by rewriting atomic physics — calculating electronic orbitals. But to just come to this conclusion, it was first necessary to identify the contradictions that arise when using standard chemical orbitals to describe the physical and chemical properties of substances.

And at the initial stage of the analysis and calculation of classical corrections of fundamental doubts about the correctness of quantum-mechanical calculations of electronic orbitals- "springs", by and large, have not yet arisen. Although the orbitals introduced by Pauling [18], based on of which two-dimensional models of graphite and boron nitride crystals were built, were noticed long ago, they contradicted several previous experiments and directly contradicted the experimentally measured anisotropy of lattice vibrations of boron nitride (see Fig. 1 ). Although even at this stage of research, a drastic difference was found in the ion-covalent bond between the two-dimensional layers of hexagons found in these crystals, only a small deformation of one of the four already known atomic orbitals formed in the BN molecule was used to correct [13].

Those. The cardinal difference between the generally accepted Van der Waals interaction and experiments was eliminated by taking into account this slightly deformed orbital, which was previously simply not taken into account in the formation of the crystal structure. And for the electronic allowed energy levels and the shape (symmetry) of the electronic orbitals obtained in the framework of the quantum oscillator model, but in the Coulomb potential of the nucleus - in the framework of the hydrogen-like atom model, in general, there was no doubt. Moreover, even at the level of the concepts of s, p, d, f orbital, there was a good, qualitative correlation of the filling of the upper electronic levels with both the ionization potentials of atoms and the physical characteristics of materials (Fig. 6).

Moreover, the experimental energy characteristics which are shown in Fig. 6 “feel” well the symmetry change of the upper occupied orbitals [20, 21] —and the complete filling of s– orbitals, and the transition from the filled $2s^2$– orbitals to the p-orbitals (jump $\Delta_1$) and filling three electrons of the p-orbital, and even the transition from a fully p-orbital to a new p-orbital too (jump$\Delta_2$). Then, formally, within the framework of the used model of a quantum oscillator in the Coulomb potential, the calculated dependence on the atomic number n of the position of the upper filled level $E^*_n$(the pink dashed curve in Fig. 6) is degenerate by the symmetry of the orbitals - the energy of the calculated level is determined (supposedly) only by the main quantum number.

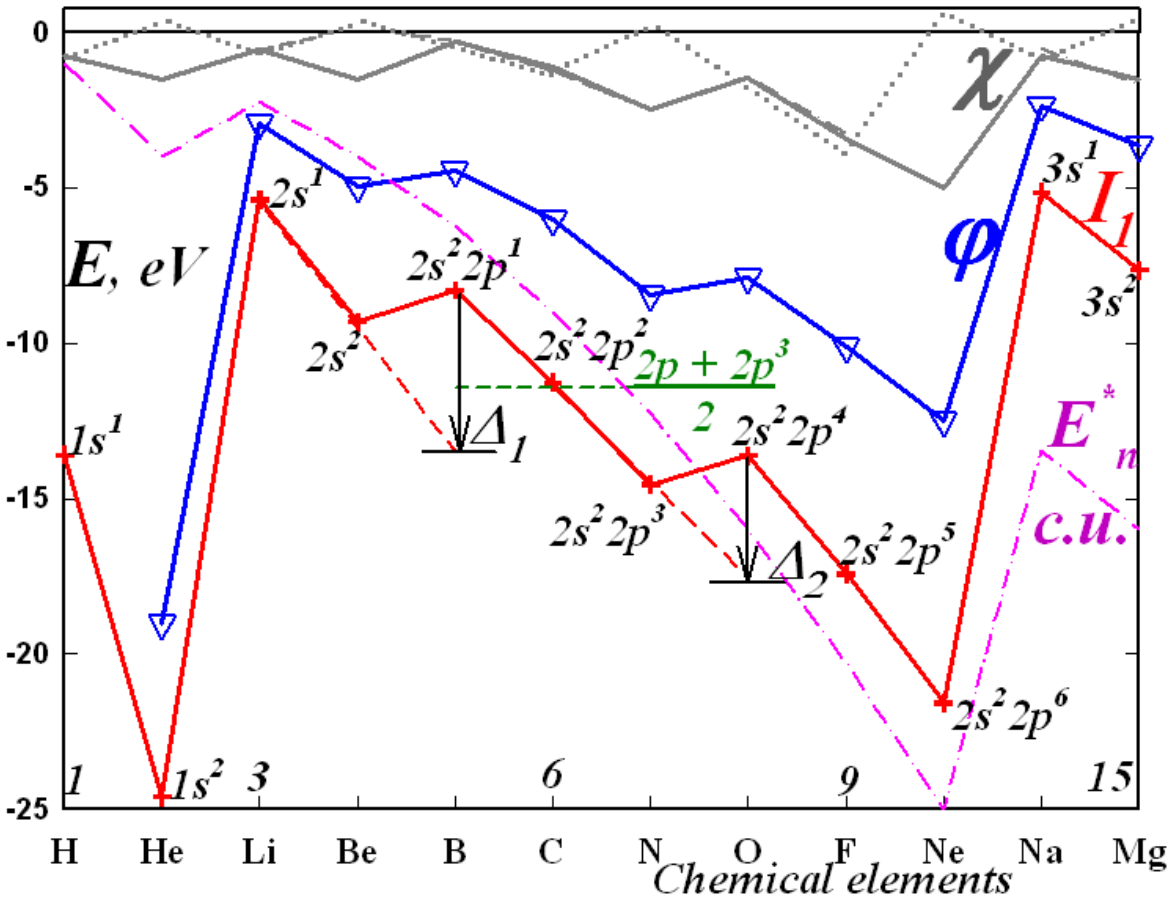


*Fig. 6:* Periodic and intraperiodic correlation of electron orbitals with the first ionization potential $I_1$, work function $\varphi$ and electron affinity of materials $\chi$

But if in the first periods the quantitative difference between the calculated energy levels with the experimentally measured energies is relatively small, then for large atomic numbers, as shown in [22 23], the discrepancy is catastrophic. Therefore, purely levels in the Coulomb potential in quantitative calculations do not use at all. Whereas a transformation similar to that shown in Fig. 4 for phonons but experimentally measured electronic levels in atoms into energy bands of allowed states in substances (Fig. 7) was experimentally repeatedly studied and described in terms of various models [24].

The algorithm for the natural broadening of the resonance band of coupled oscillators used in Fig. 7 to construct also followed from consideration of coupled classical oscillators and the transformation of the allowed upper occupied electron levels into bands was reliably established by experimental measurements of these levels in gases and their broadening upon transition to clusters and single crystals.

So the algorithm which is shown in Fig. 7 for broadening the allowed levels into zones of allowed states, similar to the broadening of the classical resonant level of ions in the band of allowed vibrations shown in Fig. 4, and in the parabolic Coulomb potential, can also be considered quite reasonable and used for practical calculations of allowed and forbidden energy zones. And in fact, this is done with numerous quantum-mechanical calculations, which is actually a calculation of corrections, acceptable only if the corrections are small. And if we do not eliminate the contradictions in their basis we have “a tree without roots”, it is often a great arbitrariness in the choice of fitting parameters by theorists and a rather cool attitude to such calculations by practitioners - technologists and experimenters.

And to break this vicious circle, we qualitatively summarize the revealed contradictions in quantum calculations, which are directly tied to ideas about electronics, in fact, chemical orbitals.

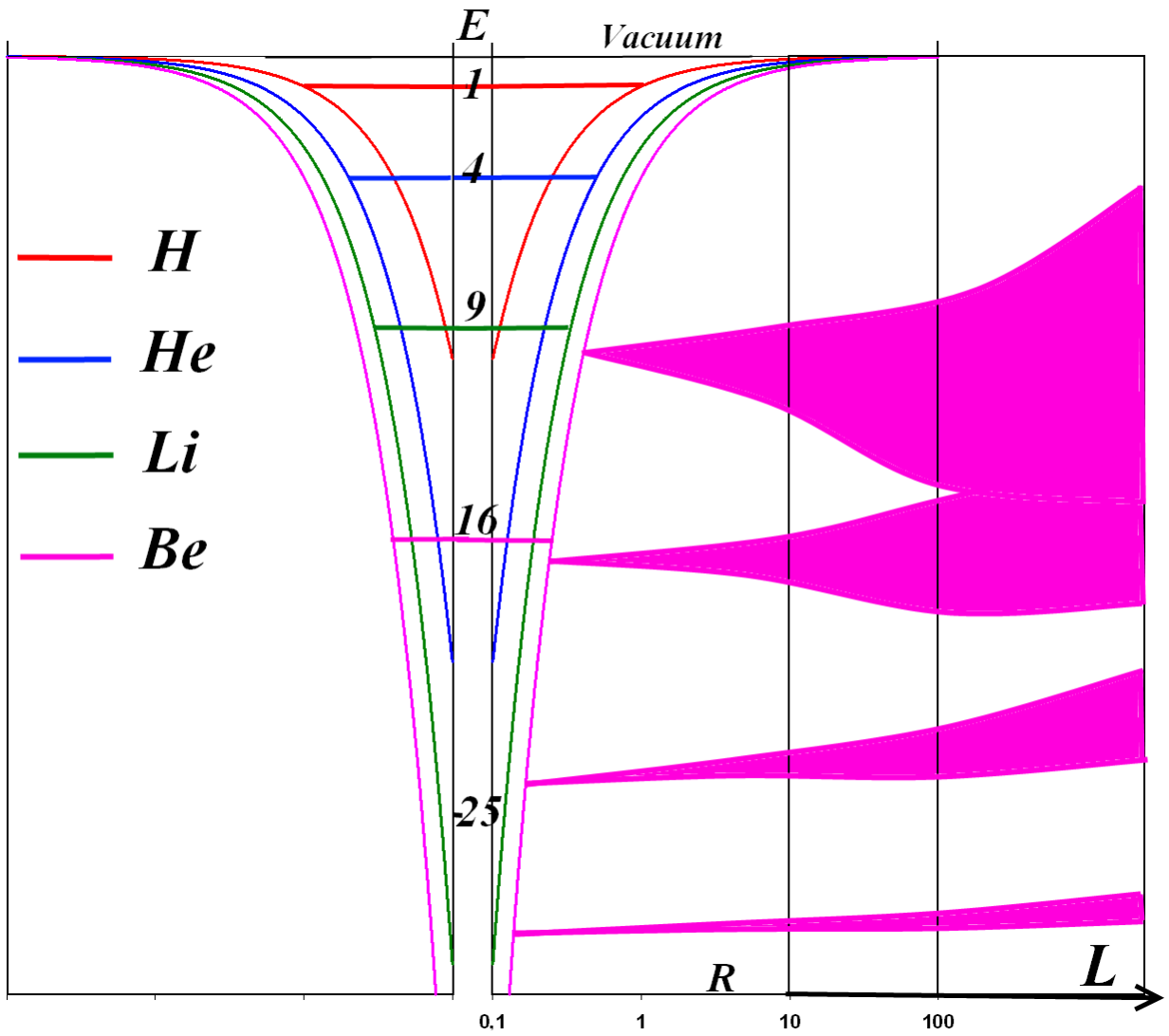


*Fig. 7:* The calculated upper levels of a row of elements in the corresponding Coulomb potential and the scheme of broadening of experimentally observed beryllium levels to allowed zones

On the other hand, the three-dimensional solutions found for electrons for hydrogen-like atoms with a centrosymmetric potential are, in principle, non-strict and incomplete, i.e., approximate. Moreover, they cannot be verified, as with dipoles in a lattice, within the framework of a clear one-dimensional model - even a qualitative consideration, as with dipoles, of a one-dimensional model, when quantized in a hydrogen-like model, is generally incorrect. And the three-dimensional wave functions obtained by the method of separation of solution variables are also not strict, qualitative, and in many respects demonstrative in nature. Nevertheless, such an approach gave a qualitative description of the entire periodic table of elements, which indicates the closeness of the obtained dependences of the wave functions on the angular coordinates to the true ones, the main error "hid" in calculating the energy from the radius! Both for electrons and, in the seemingly simplest case, for phonons.

So, let's go back to Einstein's formula: "Some equations of classical physics can be rewritten in operator form!" [25].

And we that either models (classical) that are not strictly selected for rewriting, or the algorithm for rewriting into operator form is not strict.

From the catastrophic discrepancy between the electronic levels of a hydrogen-like atom for large atoms, in principle, the conclusion made in [22] immediately follows: a hydrogen-like atom is not ELEMENTARY for all atoms, but is a kind of simplification and, in principle, as a primitive cell is NOT TRANSLATED.

But from this alone it already follows that the Schrödinger equation has not of a general nature, but a certain approximate equation for the limiting particular case.

So, the QUESTION about the Electronic Orbitals that determine the chemical bond directly related to

Chemistry returned to the Fundamentals of Quantum Mechanics.

## II. Conclusion

Applied research chemists usually just need to know that there is some kind of quantum mechanics that describes theoretically chemical bonds. But in practice, they simply use the purely chemically established these bonds in the atomic-molecular design of new substances and materials. And in many respects, they rely not on theory but on their instinct for the experimenter. Boris Nikolayevich Sharupin also had such a great instinct for the technologist, who for my research grows magnificent, highly ordered crystals of boron nitride and graphite, and for industry - excellent products from them. But this remarkable scientist (who was included in the co-authors of the article posthumously) was the first to invite me to the conference with a report refuting the decorative science, which was also given in his book. So apparently he understood that one instinct was not enough to get new materials. And this HIS understanding of the significance of Science has pushed me to deeply understand the contradictions that have accumulated in it over a hundred years. And our own understanding is that without a single picture in Consciousness (in theory), we will not get a reliable tool for practice, both for the Press and for technology.

But as shown earlier, the Schrödinger equation, on which almost all quantum-mechanical calculations are based, not only describes the hydrogen atom, but non-invariant and gives catastrophic discrepancies for all other atoms, which are trying to "correct" by approximation methods. A fundamental "correction" required both the elimination of Schrödinger's error in comparing the difference in size and the correction of the "kKantivanie" itself, continued contrary to Planck's ideas.

Quantization Max Planck, in principle, calculated for the electromagnetic field. And, following strictly Planck, it was necessary to initially build Quantum Electrodynamics on the basis of electrical models. Or at least Quantum NONMECHANICS or Quantum ELECTROMECHANICS. And naturally on the basis of electrical models, in particular, on the basis of a well-describing electrical impedance measurement results.

But this will be discussed in detail in the following works: "Impedance of the Skin-Plasma Effect" and "Quantum Non-Mechanics"

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# Synthesis and Research of New Compounds of Guanidine on the Basis of α-Chlorether and Chlorazone

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*Baku State University*

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*Keywords: guanidine, α- chloroesters, alcohol, chlorazone, synthesis, research, ecological, inhibitor, corrosion, aggressive environment, oil and gas, petrochemical industry, steel, technological equipment.*

*GJSFR-B Classification: FOR Code: 250399*


*Strictly as per the compliance and regulations of:*

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S. R. Hajiyeva [α], G. I. Bayramov [σ], F. E. Huseynov [ρ], T. I. Aliyeva [Ω], H. L. Rafiyeva [¥], Z. T. Valiyeva [§], A. A. Samadova [χ] & N. M. Jafarova [ν]

*Abstract-* The reactions of chlorazone with α-chloroethyl esters of n-$C_8H_{17}OH$, n-$C_{10}H_{21}OH$, n-$C_{12}H_{25}OH$, $CH_3$-CH=CCl-$CH_2OH$ alcohols for the first time were carried out, and chlorazone esters containing two $ROCH_2$ groups of these esters were obtained. The reactions of $N_1$-alkoxymethyl-$N_3$-alkoxy-methylguanidine compounds with these chlorazone esters were carried out and 4 new guanidine derivatives (conventionally designated as I-IV) were synthesized, not known in the literature. Studies have been conducted to establish corrosion inhibitory efficiency for each of the newly synthesized compounds of guanidine I-IV in a very strong aggressive environment created in the laboratory. It was established that the inhibitory effectiveness of these compounds in concentrations of 1.0; 2.0; 2.5 mg/l is 99.97-100%. A comparative study of the effective inhibitory properties of the new synthesized guanidine compounds for corrosion protection of steel "St.3" was carried out. Studies have shown that each of the new I-IV compounds of guanidine in terms of environmental safety, economic and environmental efficiency is 5-10 times higher than the inhibitors currently used to protect from corrosion steel processing equipment operating in aggressive environments.

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## I. Introduction

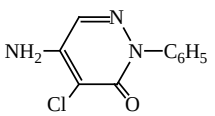
Based on the technical data and the results of our previous studies, it was established that organic compounds containing nitrogen atoms, - $CH_2$ -, $ROCH_2$ groups and other functional groups, many double bonds possess highly effective inhibitory properties[1].

Therefore, the synthesis and study of this type of compound is considered as one of the most relevant topics in organic chemistry, petrochemistry and ecological chemistry.

In this direction, initially with the use of n-$C_8H_{17}OH$, n-$C_{10}H_{21}OH$, n-$C_{12}H_{25}OH$ alcohols, considered to be a cheap raw material and $CH_3$-CH=CCl-$CH_2OH$ alcohol from the production of synthetic rubber $CH_3$-CH=CCl-$CH_2Cl$ (1,2-dixlorbuten-2), as well as $CH_2O$ (paraform), α-chloro esters of these alcohols were synthesized.

We give a brief overview of the raw materials (chemical compounds) used for the synthesis of new guanidine compounds.

1. n-$C_8H_{17}OH$(normaloctylalcohol)octanol-1, belongs to the class of high molecular weight alcohols, has a floral-citrus aroma (orange, etc.), is poorly soluble in water, well soluble in ethanol, is in a liquid state of aggregation, molecular weight 130.23 g / mol;$\rho_4^{20}$ = 0.824 g / $cm^3$, $t_{boil}$ = 195°C, rat dose "$LD_{50}$"> 5 g / kg, MPC = 10 mg / $m^3$.
2. n - $C_{10}H_{21}OH$ (normal decyl alcohol) decanol-1, belongs to the class of fatty alcohols, molecular weight 156.27; colorless liquid, it has the aroma of roses, $\rho_4^{20}$ = 0.8297 g / $cm^3$, $n_D^{20}$ = 1.4372, $t_{boil}$ = 229°C, it is well soluble in ethanol.
3. n-$C_{12}H_{25}OH$ (normal dodecyl alcohol) $CH_3$ $(CH_2)_{10}CH_2OH$ or $C_{12}H_{25}OH$, $\rho_4^{20}$= 0.8201 g / $cm^3$, $n_D^{20}$ = 1.4455, molar mass 186.34 g / mol, colorless, low-viscosity liquid with a floral-citrus aroma (lemon, orange, tangerine), $t_{boil}$ = 259 ° C.
4. Compound$CH_3$-CH=CCl-$CH_2Cl$(1,2-dichlorobutene-2)(low molecular weight formaldehyde polymer, mixture of polyoxymethylene glycol), general formula [-$CH_2O$-] x, HO - [- $CH_2O$] xH x = 8 colorless or in the form of white crystals substance, mp = 120-170 ° C.
5. $CH_3$-CH=CCl-$CH_2OH$ (2-chlorobutene-2-ol-1) alcohol, $\rho_4^{20}$=1,1060;$n_D^{20}$=1,4712,$t_{boil}$= 49-50°C / 50 mm Hg, a liquid with a pungent unpleasant odor, is well soluble in water, ethyl alcohol, benzene and toluene.
6. ($CH_2O$) n (paraform compound) low molecular weight formaldehyde polymer, mixture of polyoxymethylene glycol), general formula [-$CH_2O$-] x, HO - [- $CH_2O$] xH x = 8 ÷ 100; colorless or in the form of white crystals substance, mp = 120-170° C.

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7. Chlorazone(1-phenyl-4-amino-5chloropyridazone-6) $C_{10}H_8ClN_3O$, mp = 202 ° C, a substance in the form of white crystals, is dissolved in $CH_3OH$, a low-toxic substance (rat dose "$LD_{50}$" - 3600 mg / l), standard «СЭВ1052-78».

The raw materials mentioned above were used after determining their $d_4^{20}$, $n_d^{20}$ constants and boiling points.

α-Chloroctoxymethyl($C_8H_{17}OCH_2Cl$), α-chlordecoxymethyl ($C_{10}H_{21}OCH_2Cl$), α-chlordodecoxymethyl ($C_{12}H_{25}OCH_2Cl$), α-chlor-2-chlor-5-oxohexane-2 ($CH_3$-CH=CCl-$CH_2O$ $CH_2Cl$) esters and obtained on the base of this esters $ROCH_2$-NH-C-NH-$CH_2OR$ compounds and ($N_1'$,$N_1'$-dialkoxymethylchlororazone) esters [2-4] were synthesized according to the methods described in the literature.

The composition and structure of each of the aforementioned α-chloroesters, $N_1'$,$N_1'$-dialkoxymethyl-chlororazone, and $N_1$-alkoxymethyl-$N_3$-alkoxymethylguanide compounds synthesized in several stages were determined by known methods.

The IR-spectra of the compounds obtained by the reaction of guanidine and α-chloroalkoxymethyl esters in step III are shown, for example, in Fig. 1.

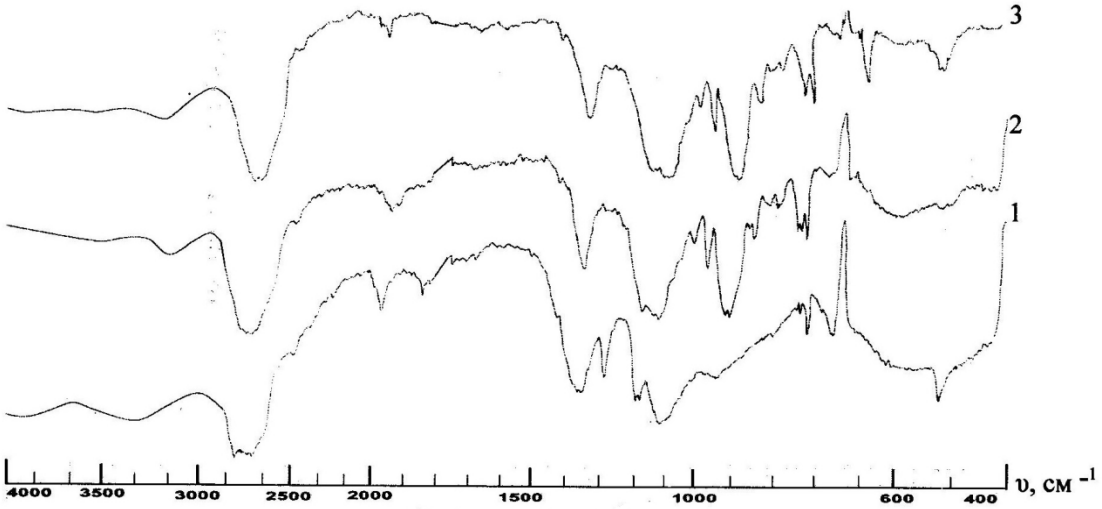



*Fig. 1:* 1- IR-spectra of the compound of raw materials of guanidine, 2 - compound of $N_1$-octoxymethyl-$N_3$-octoxymethylguanidine, 3 - compound of $N_1$- (2-chlor-5-oxohexene-2) -$N_3$- (2chlor-5-oxohexene-2) guanidine

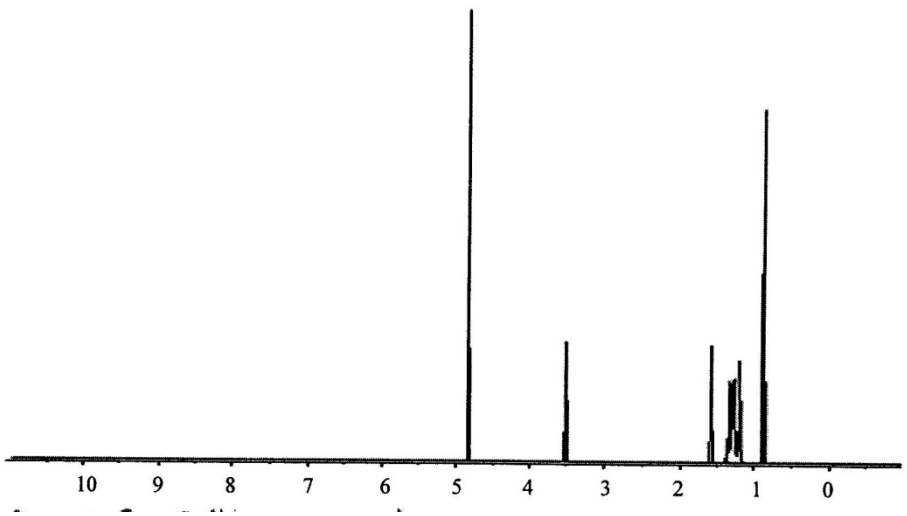



*Fig. 2:* NMR H spectrum of the compound $N_1$-octoxymethyl-$N_3$octoxymethylguanidine

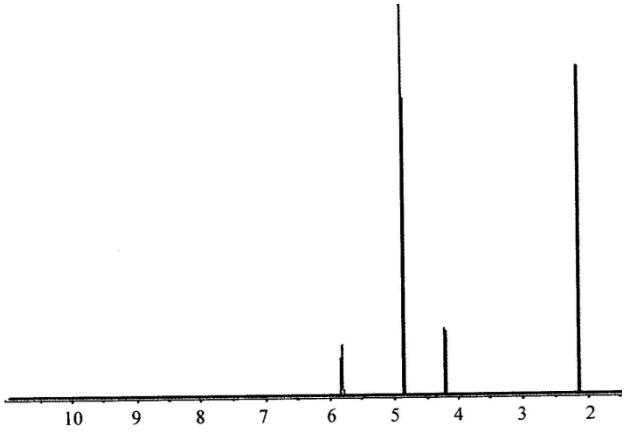
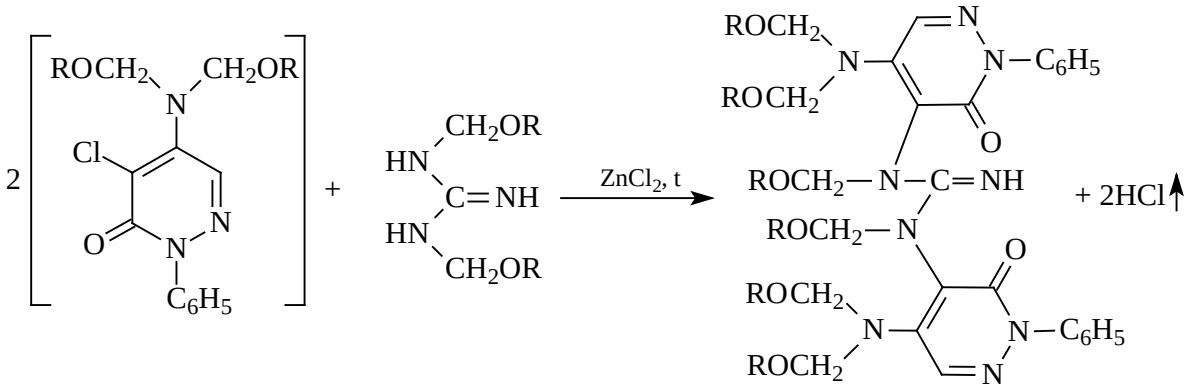



*Fig. 3:* NMR H spectrum of the compound $N_1$- (2-chlor-5-oxohexene-2) -$N_3$- (2 chlor-5-oxohexene-2) guanidine

At the fourth stage, the reactionwith $N_1$-alkoxymethyl-$N_3$-alkoxymethylguanidone organic compounds and new derivatives of guanidine were synthesized (compounds I – IV). The synthesis was carried out by a known method in the literature [3]

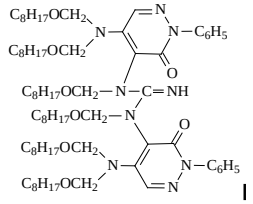
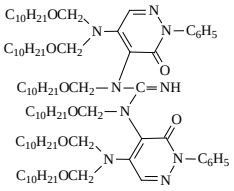
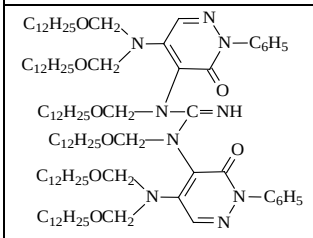
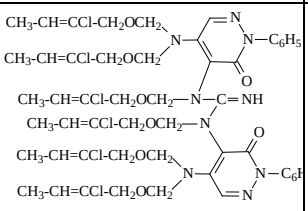



where; R= $–C_8H_{17}$ (I); $–C_{10}H_{21}$ (II); $–C_{12}H_{25}$ (III); $–CH_2–CH=CCl–CH_3$ (IV).

The structure of new synthesized organic compounds I–IV was determined by registering their IR-, mass- and NMR spectra. Information on this is presented in the experimental section.

Percentage yield, physico-chemical constants and elemental analysis of new guanidine derivatives (compounds I - IV) are shown in Table 1.

*Table 1:* Percentage yield, physico-chemical constants and elemental analysis of synthesized new I - IV compounds of guanidine based on α-chloroesters and chlorazone

| Chemical formula and Conditional Compound Number | Yield, % | $T_{boil}$, °C (mm Hg) | $d_4^{20}$ | $n_D^{20}$ | $MR_D$ found / calculated | Gross formula, mol. weight | Elemental analysis, % Calculated / Found | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | C | H | N | Cl |
|  I | 98,75 | 320-321 (3) | 1,1580 | 1,6115 | 384,29 / 384,17 | $C_{75}H_{127}N_9O_8$ 1281 | 70,25 / 69,87 | 9,91 / 9,67 | 9,84 / 9,58 | - |
|  II | 98,65 | 335-336 (3) | 1,1601 | 1,6225 | 410,16 / 439,93 | $C_{87}H_{151}N_9O_8$ 1449 | 72,05 / 71,92 | 10,42 / 10,21 | 8,69 / 6,54 | – |
|  III | 98,47 | 350-351 (3) | 1,1661 | 1,6315 | 494,92 / 494,70 | $C_{99}H_{175}N_9O_8$ 1617 | 73,47 / 73,16 | 14,73 / 14,51 | 7,79 / 7,54 | – |
|  IV | 96,24 | 365-366 (3) | 1,4108 | 1,6615 | 298,84 / 298,63 | $C_{51}H_{61}N_9O_8C_6$ 1140 | 53,68 / 53,42 | 5,32 / 5,04 | 11,05 / 10,8 | 18,68 / 18,2 |

## II. Experimental Part

*a) Synthesis of $N_1$-(octoxymethyl-N', N'-dioctoxymethyl) -$N_3$- (octoxymethyl-N', N'-dioctoxymethyl) guanidine ((compound I).*

In a synthesis flask, 2 g of $ZnCl_2$, (0.01 g-mol) of $N_1$-octoxymethyl-$N_3$'-octoxymethylguanidine are placed and 100 ml of ethyl alcohol is added, stirring heated to 70°C. Then (0.02 g-mol) of $N_1'$,$N_1'$-dioctoxymethyl chlorononе ester is gradually added to the mixture. Stirring is continued for 6 hours at the alcohol condensation temperature. After that, at room temperature, 100 ml of 10% NaOH solution is added to the reaction flask, stirred for 0.5 h, 200 ml of distilled water are added. The organic layer is extracted with diethyl ether, and after the distillation of the ether, it is dried over $CaCl_2$. The residue is distilled in a vacuum unit with the release of synthesis of $N_1$-(octoxymethyl-$N_1'$,$N_1'$-dioctoxymethylazone) -$N_3$-(octoxymethyl- $N_1'$,$N_1'$-dioctoxymethylazone) guanidine (I), which is a yellow, viscous liquid with a strong specific odor.

Similarly were synthesized $N_1$-(decoxymethyl-$N_1'$,$N_1'$-dideoxymethylazone) -$N_3$- (decoxymethyl-$N_1'$, $N_1'$-dideoxymethylazone) guanidine (compound II), N1-(dodeoxymethyl-$N_1'$,$N_1'$-dimethode)–$N_3$-(dodeoxymethyl-$N_1'$,$N_1'$-didodecoxymethylazone) guanidine (compound III) and $N_1$-[(2-chlor-5-oxohexene-2)-$N_1'$,$N_1'$-di(2-chlor-5-oxohexene-2)azone]-$N_3$-[(2-chlor-5-oxohexene-2-) $N_1'$, $N_1'$-di (2-chlor-5-oxohexene-2) azone] guanidine (compound IV).

The compositions and structures of the synthesized compounds I- IV were established on the basis of the data of elemental analysis, IR-, mass-, and NMR spectra.

In the mass spectra of compounds I-IV, it was determined that their molecular masses correspond to molecular ions 1449 m/e, 1617 m/e and 1140 m/e.

In IR-spectrum of comp. IV, the ether group C-O-C 1050, 1080 $cm^{-1}$ appears as an intense band; bond C-N 1310-1350 $cm^{-1}$; $CH_2$ group 2950 $cm^{-1}$; $CH_3$ group 1380, 1400, 1460, 2990, 3030 $cm^{-1}$; NH group 2910, 3113, 3340, 3360, 3400, 3450 $cm^{-1}$; belonging to the

group of azone C = C bond 1680 $cm^{-1}$; in the benzene ring C = C bond 1440-1465,1500-1510, 1590-1600 $cm^{-1}$;$C_6H_5$ group 700-780 $cm^{-1}$,C – Cl bond 680 $cm^{-1}$.

In the NMR spectra of compounds I- IV singlets at 3.94–4.40 ppm.and 4.75-5.55 ppm correspond to the protons of the methylene groups of the fragments > N–$CH_2$ – and > N–$CH_2$ – O.

The NMR spectra of the I- IV compounds contain signals of the methylene groups of the ring (wide intense multiplet in the region of 1.41-1.82 ppm), the methyl group (a triplet of 0.8-1.21 ppm), the group - $CH_2O$ - (doublet 2.05 ppm). In the range of 6-8 ppm two doublets correspond to signals of two non-equivalent m-protons of the benzene ring of the I- IV compounds and not changing their position when strongly diluted indicates a strong C = N-hydrogen bond also (2H, -C-N-$CH_2O$-); groups 3,45-3,47d.; 1,20-1,40 d., 1,50-1,56 d., which confirms the structure of the synthesized I- IV compounds.

Figures 4.5 show the NMR spectra of I- IV compounds

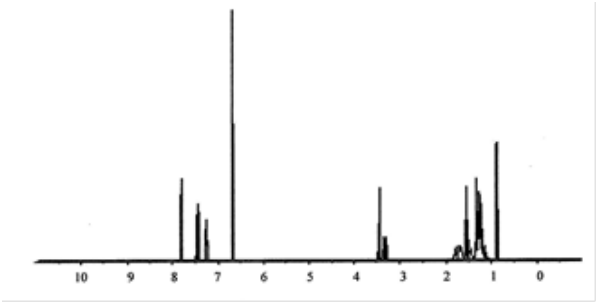



*Fig 4:* NMR spectrum H of comp. I

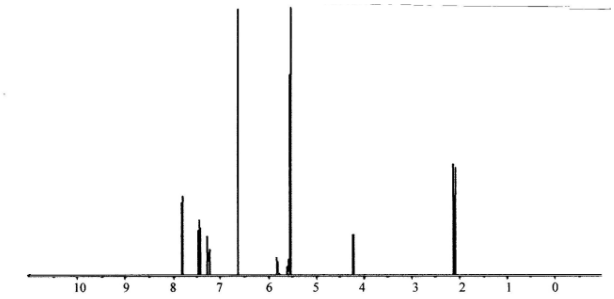



*Fig 5:* NMR spectrum H of comp. IV

## III. Discussion of the Results

To determine the inhibitory effectiveness of the synthesized new derivatives of guanidine (new compounds I - IV), studies were conducted in the literature [2-4]. In order to determine the inhibitory effectiveness of the new compounds I - IV, very corrosive media were created under laboratory conditions[3% NaCl +oil (1:10) + $H_2S$ 500 mq/l; 0,3N HCl + petrol (1:7)+ $H_2S$ 1000 mq/l].

Indicators of the inhibitory effectiveness of these compounds in the determination period are shown in table 2.

*Table 2:* The results of the study of the inhibitory efficiency of the synthesized new guanidine derivatives (new compounds I – IV)

| Conventional number of the compound | Inhibitor concentration, mg / l | 3% NaCl+oil (10:1) $H_2S$ 500 mg/l | | 0.3 N HCl + gasoline (1:7) $H_2S$ 1000 mg/l | |
|---|---|---|---|---|---|
| | | Corrosion rate, g/$cm^2$·hour | Effectiveness of the inhibitor,% | Corrosion rate, g/$cm^2$·hour | Effectiveness of the inhibitor,% |
| Without inhibitor | – | 2.56 | – | 3.65 | – |
| V | 1,0<br>2,0<br>2,5 | 0.0006<br>0.0003<br>0.0001 | 99.97<br>99.98<br>100 | 0.0061<br>0.0042<br>0.0001 | 99.83<br>99.89<br>100 |
| VI | 1,0<br>2,0<br>2,5 | 0.0003<br>0.0002<br>- | 99.98<br>99.99<br>100 | 0.0042<br>0.0015<br>– | 99.89<br>99.95<br>100 |
| VII | 1,0<br>2,0<br>2,5 | 0.0003<br>– | 99.98<br>100 | 0.002<br>0.0008<br>– | 99.94<br>99.98<br>100 |
| VIII | 1,0<br>2,0<br>2,5 | – | 100 | 0.0008<br>-<br>– | 99.98<br>100 |
| A [4] | 200 | | 98.5 | | 98 |

As can be seen from table 2, each of the synthesized new derivatives I - IV at a concentration of 1; 2; 2.5 mg/l possesses 100% inhibitory activity and exceeds in its qualities the compound known in the literature [4], which obtained the author's certificate and was conditionally called by us compound A, even at its high concentration. And also in the literature [13] was named IFKHAN-92, a high-temperature (up to 140 $^0$C) corrosion inhibitor for steel in $H_2SO_4$ solutions, providing an efficiency of Z = 99%, with a content of less than 1% of the mass.

According to [7], the effectiveness of inhibitors of the "AMDOP-IR-7" type increases with increasing concentration of hydrogen sulfide and deoxygenation of the medium. In some cases, the function Z = f ($C_{hydrogen\ sulfide}$) passes through a maximum. This again was confirmed by studies conducted by us.

In order to elucidate the mechanism of the protective action and predict the effectiveness of inhibitors in many of the research studies developed, it was proved that molecules with only one functional group exhibit weak inhibitory properties, if in them there are two such groups, the inhibitory effect is sharply enhanced [2-4; 5-11].

Based on the requirements presented in the literature [12], multifunctional reagents, inhibitors must meet environmental safety. Based on the above, we have synthesized new organic nitrogen-containing compounds that meet all these requirements. It appears that the presence of double bonds, multifunctional groups —$CH_2OR$ and nitrogen atoms in the composition of new compounds I - IV and an increase in the electron density contribute to the formation of a complex between the inhibitor molecule and the metal on the steel surface, creating a high adsorption and the steel surface becomes passive to corrosion.

Based on the conducted research, it can be considered that the synthesized new guanidine derivatives (new compounds I - IV) can be used as inhibitors in the oil-gas producing, oil refining and petrochemical industries to protect steel technological equipment from corrosion and can guarantee high both economic and environmental efficiency.

As can be seen from the compositions and structures of new guanidine derivatives (new compounds I - IV), these compounds can find their use as additives, biologically active substances, insecticides, flotation reagents, as well as in other directions.

From the above mentioned it follows that the synthesis of compounds of this type and their research in the synthesis of organic chemistry can be assessed as very relevant.

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# Potassium Iodate ($KIO_3$)-A Novel Reagent for the Dehydrogenation of Cyclohexanone

By Harinakshi, Rashmi, Yashika, Balakrishn Kalluraya, Nagma & K. M. Lokanatha Rai
*Mangalore University*

*Abstract-* Anovel reagent for the dehydrogenation of cyclohexanone has been reported. Cyclohexanone was made to react with a novel reagent – $KIO_3$ as oxidizing agent in presence of acetic acid. The dehydrogenated compound was confirmed by comparison with the known compound. This metal free process is less time consuming and the easy availability and its stability makes it a versatile novel reagent for the dehydrogenation of cyclohexanone.

*GJSFR-B Classification:* *FOR Code: 250499*


*Strictly as per the compliance and regulations of:*

# Potassium Iodate ($KIO_3$) - A Novel Reagent for the Dehydrogenation of Cyclohexanone

Harinakshi [α], Rashmi [σ], Yashika [ρ], Balakrishn Kalluraya [ω], Nagma [¥] & K. M. Lokanatha Rai [§]

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## I. Introduction

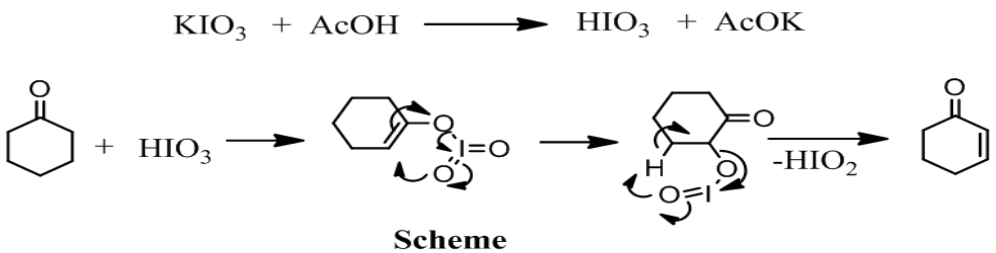
The conversion of ketones to the more versatile enone functionality is an important transformation in organic synthesis due to the utility of enones as intermediates in multistep production of pharmaceuticals and biologically active compounds. One of the earliest strategies for the synthesis of enones involves the pre-functionalization of the ketone a-position with a halogen, which can be eliminated upon treatment with base at high temperatures.[1] Utilizing aselenide intermediates is similarly broad in scope as these species can be formed under mild conditions through trapping of a lithium enolate with PhSeX.[2] The second step entails conversion of the selenide moiety to the corresponding selenoxide, which allows for spontaneous generation of aunsaturated products via a 2,3-sigmatropic rearrangement.[3]

Literature survey revealed $KIO_3$/KI in acetic acid is used as iodination agent at 110°C.[4]Combination of iodic acid and potassium iodide has been used for trimethylsilylation of alcohols and phenols in the presence of HMDS and iodination of aromatic amines[5]. Recently Kelsey B. LaMartina et al showed that the combinations of ammonium iodate and catalytic *N*-hydroxyphthalimide (NHPI) in presence of acetic acid for the selective oxidation of *n*-butylbenzene directly to 1-phenylbutyl acetate in high yield[6] and it is also reported as catalyst for the α-sulfenylation of enaminones[7]. Recently Rai *et al* used $KIO_3$ as a novel oxidising agent for the synthesis of isoxazolines[8].

This prompted us to use this reagent for the dehydrogenation of cyclohexanone. This metal free process is less time consuming and the easy availability and its stability makes it a versatile novel reagent for the dehydrogenation of cyclohexanone. Further applications of this novel reagent are under progress.

Typically the dehydrogenation is carried out by heating equimolar mixture of cyclohexanone, potassium iodate and acetic acid in ethanol under reflux for 4-6 hrs. The dehydrogenated compound was confirmed by comparison with the known compound.

Probable mechanism is given in Scheme. The reaction involves the protonation of cyclohexanone followed by enolization and esterification leads to enol ester. This ester undergoes rearrangement to give α-keto ester, followed by cis elimination of $HIO_2$ leads to the formation of cyclohexenone in almost quantitative yield.




**Scheme**

## II. Experimental

*a) Dehydrogenation of cyclohexanone*

In a typical procedure cyclohexanone was to react with a new reagent $KIO_3$(1.2mmol) as oxidizing agent under reflux conditions for 4-6hours in the presence of acetic acid in catalytic amount and ethanol as solvent. The completion of the reaction was monitored by TLC. After completion, the residue was extracted with ether (25mL×3), the extract was washed successively with water (15mL×2), 10% NaOH

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(15mL×2), and saturated brine solution (10mL).The organic layer was dried over anhydrous $Na_2SO_4$.

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By Adel H. Ali
*Taiz University*

*Abstract-* The rule of this paper is to study a possibility of using Simvastatin pharmaceutical drug compound as corrosion inhibitor that can have a decisive effect of decreasing on metallic corrosion rate and adsorbed on the metal surface by using potentiodynamic polarization and Evans techniques. In this regard, we simultaneously present an overview on Simvastatin compound performance, as corrosion inhibitor in 10% ethanol, 0.5N $H_2SO_4$ (10A5H), and with presence different concentration of drug. The potentiodynamic polarization and Evans technique are studied the LCH in different medium to clarify the effect of medium on the corrosion processes and the effect of polarization on the orientation of inhibitor molecule to the metal surface. The surface examination by scanning electron microscopy (SEM), energy dispersive X-ray (EDX) and atomic force microscopy (AFM). All surface examinations confirm formation, thin film adsorbed on the metal surface which discussed by the mechanism of the adsorption processes on the polarized metal surface.

*Keywords: corrosion inhibition; potentiodynamic polariza-tion; Evans technique; mixed solution (10A5H); Simvastatin inhibitor; SEM; EDX; AFM.*

*GJSFR-B Classification: FOR Code: 030699*

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## I. Introduction

Most organic compounds containing nitrogen (N-heterocyclic), sulfur, long carbon chain or aromatic and oxygen atoms. Among them, organic compounds have many advantages such as: high molecular size, highly soluble in water, availability, cheap, low toxicity, easy for using and easy production[1]. Natural heterocyclic mixes have been utilized for the corrosion inhibitor on the C-steel [2], copper [3], aluminum [4], and various metals in various aqueous medium [5]. Adsorption of the drug molecules on the metal surface facilitates its inhibition[6]. The investigation of the relations between the adsorption and consumption hindrance is of awesome important. Heterocyclic mixes have demonstrated more hindrance effectiveness for C-steel in both HCl [7] and $H_2SO_4$ arrangements[8]. Numerous authors for the most part concur that medications are inhibitors that can compete favorably with green inhibition of corrosion and that most medications can be synthesized from natural products. Selection of some medication as corrosion inhibitors due to the followings: (1) drug molecules contain oxygen, sulphur and nitrogen as active sites, (2) it is environmentally friendly furthermore vital in organic responses and (3) drugs can be easily produced and purified (4) nontoxic compering organic inhibitors. A few medications have been discovered to be great corrosion inhibitors for metals such as: Biopolymer gave 86% IE for Cu in NaCl[9], pyromellitic diimide linked to oxadiazole cycle gave 84.6% IE for MS in HCl[10], 2-mercaptobenzimidazole gave 82% IE for MS in HClAntidiabetic Drug Janumet gave 88.7% IE for MS in HCl [11]. Januvia gave 79.5 % IE for Zn in HCl [12], Cefuroxime Axetil gave 89.9% IE for Al in HCl [13], Phenytoin sodium gave 79% for MS in HCl [14], Aspirin gave71% IE for MS in $H_2SO_4$[15], Septazole gave 84.8% IE for Cu in HCl [16] and Chloroquine diphosphate gave 80% IE for MS in HCl [17]. Study on Structural, Corrosion, and Sensitization Behavior of Ultrafine and Coarse Grain 316 Stainless Steel Processed by Multiaxial Forging and Heat Treatment [18]. Investigating the corrosion of the Heat-Affected Zones (HAZs) of API-X70 pipeline steels in aerated carbonate solution by electrochemical methods[19]. Predictions of corrosion current density and potential by using chemical composition and corrosion cell characteristics in microalloyed pipeline steels [20]. Predictions of toughness and hardness by using chemical composition and tensile properties in microalloyed line pipe steels[21].

The scope of this article is to use Simvastatin drug as save corrosion inhibitor for LCH in acid medium by electrochemical method, and to elucidate the mechanism of corrosion inhibition.

## II. Experimental

### a) Metal samples

Two samples of carbon steel was used in the study that have the chemical composition of the metal

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samples was determined using emission spectrometer, with the aid of ARL quant meter (model 3100-292 IC) and listed in the Table 1.

*Table 1:* Chemical compositions of carbon steel sample

| Sample | C% | Mn% | V% | Fe% | Si% |
|---|---|---|---|---|---|
| Low; C | 0.26 | 0.77 | 0.11 | 98.51 | 0.35 |

*b) Quenching in oil*

The used heat treatment regime was Quenching in oil. As-received sample was putting in an electric muffle furnace where the raising temperature is 920 °C (Austentizing temperature) through five hours. Then, the sample remains in furnace for one hour at 920°C, (Holding time), followed quenching of sample in oil.

The phase, which formed due to these heat treatment sampleis converted from ferretic phase to martensite phase[22].

The steps of this regime are shown diagrammatically in Figure 1.

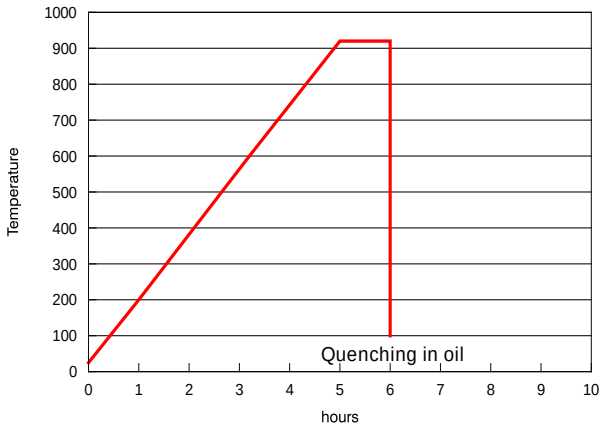


*Figure 1:* Heat treatment regime

*c) Preparation of metal sample (working electrode)*

The working electrode having the surface area, which, exposed to corrosion media is (1$Cm^2$) cross-section area and the rod was weld from one side to a copper wire used for electric connection. The sample was embedded in glass of just larger diameter than the sample. Epoxy resin was used to stick the sample to glass tube. These also insured that constant cross-sectional area would be exposed to corrosive media through the experiments. The sample was scraped with SiC polisher sheet coarseness sizes (400, 800 and 1200) and clean with (CH3)2CO. At that point, clean a few times with bi-distilled water, lastly dried by soft tissue. Finally polishing of sample surface to be mirror bright, just before immersion in the electrolyte cell.

*d) Simvastatin drug as an inhibitor*

The Simvastatin ($C_{25}H_{38}O_5$) inhibitor have molecular mass (418.566 g/mol) which containing 5 oxygen atoms and$\pi$2bonding that acts as active centers. The unshared electrons of oxygen atoms and the electron density of $\pi$-bonding acts donor site to the anodic sites of the metal surface.

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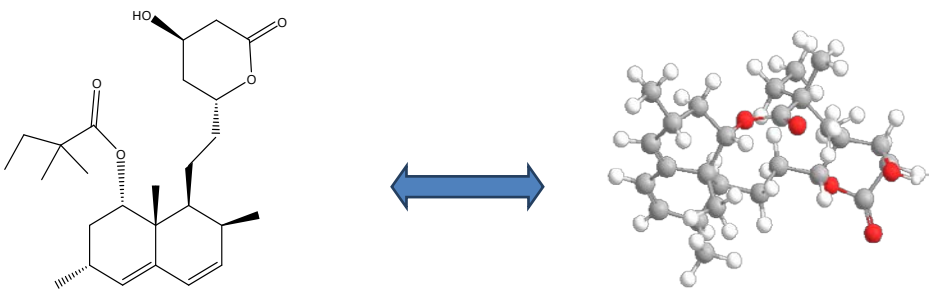



(1S,3R,7S,8S,8aR)-8-(2-((2R,4R)-4-hydroxy-6-oxotetrahydro-2H-pyran-2-yl)ethyl)-3,7,8a-trimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl 2,2-dimethylbutanoate

*e) Solutions*

A stock solution of Simvastatin was prepared by dissolving 0.0419gmSimvastatin in one liter [0.5N $H_2SO_4$ in 10% ethanol-water] to obtain $10^{-4}$ M Simvastatin solution. This stock solution then diluted by [0.5N $H_2SO_4$ in 10% ethanol-water] to prepare desired other solution. These solutions were used as corrosion medium.

This mixed solution used corrosive media and add the different of concentrations of Simvastatin (2, 4, 6, 8 and $10^{-5}$) to the corrosive media at different temperatures (15, 25, 35, 45 and 55°C).

*f) Potentiodynamic polarization measurement[23]*

Cathodic and anodic polarization technique was used for determination of corrosion rate. The electrochemical cell consists of three electrodes:

1. Platinum electrode (as a auxiliary electrode).
2. Calomel electrode (as the reference electrode). ($Hg_{(l)}$ | $Hg_2Cl_{2(s)}$, $KCl_{(aq)}$sat,) E= - 241 mV at 25°C.
3. The working electrode is LCH sample. The electrolytic cell was filled with 100 ml of the solution. The samples were immersed in the medium, then the circuit is shorted and the cathodic polarization is firstly measured by reverse the current direction the anodic polarization is measured.

*g) Calculation of rate of corrosion*

The anodic and cathodic polarization is measured by using over-potential cell. The corrosion current density ($I_{corr}$), the corrosion potential ($E_{corr}$) and the corrosion rates (R) are calculated according to Tafel extrapolation method[24].

It is clear that extrapolating the line representing the Tafel region in either cathodic or anodic polarization curve to the corrosion potential will give corrosion current density ($I_{corr}$), which can be used to calculate the corrosion rate from the equation [25-26].

$$\text{Corrosion rate (mpy)} = 0.1288\ I\ (\text{mA/cm2})\ \text{Eq.wt}\ /d\ (\text{g/cm3}) \quad (1)$$

Where, Corrosion rate (mpy) = mils per year,I= the corrosion current density,d = Specimen density, and,Eq.wt = Specimen equivalent weight.

The corrosion current density ($I_{corr}$), corrosion potential ($E_{corr}$) and corrosion rate are recorded in Table 7.

*h) Applied Evans technique*

The rate of corrosion can be understood from a graphical superposition of current-potential curves. The Evans diagrams give good and suitable interpretation about the electrode-electrolyte interface reactions. We can use the following definitions for the items of Evans diagram as follows[27]:

1- $\Delta\phi_{e,m}$ and $\Delta\phi_{e,so}$ are anodic and cathodic potentials at equilibrium at the electrode-electrolyte interface (at I =the exchange current $i_o$) respectively, where $\Delta\phi e,x = E_{e,x} \pm |E_c - E_a| i=i_o$ ; m= metal, so= solution,

2- $\Delta\phi = \Delta\phi_{corr}$ = the relative corrosion potential determined from the position of the intersection of the two curves (de-electronation and electronation processes) where, I considered as $i_{corr}$.

3- The anodic- potential difference at equilibrium (a.p.d,e) $\Delta\phi'_m = \eta_m = \Delta\phi_{corr} - \Delta\phi_{e,m}$.

4- The cathodic- potential difference at equilibrium (c.p.d,e) $\Delta\phi'_s = \eta_{so} = \Delta\phi_{corr} - \Delta\phi_{e,so}$.

5- The anodic-potential difference (a.p.d) $\Delta\phi'_a = (\Delta\phi_a)_x - (\Delta\phi)_b$ ; b =bulk, x = with additive, at different concentrations or at different temperatures, and $\Delta I_a = (i)_b - (I)_x$.

6- The cathodic-potential difference (c.p.d) $\Delta\phi'_c = (\Delta\phi)_b - (\Delta\phi_c)_x$ ; b=bulk, x= with additive, at different concentrations or at different temperatures, and $\Delta I_c = (i)_b - (I_c)_x$.

These data can be used for kinetic calculations and to know which additive is favorable or which is faster to the electrode surface at the same conditions. It can be used for studying the inhibition mechanism and aids in the classification the additives.

*i) Surface Examinations[28]*

The morphology of the LCH surface used for analysis and examination nature of the surface and study the changing that appeared on the metal surface. The specimens were prepared by abraded mechanically by using different emery papers up to 1200 grit size and immersed in (10A5H) (blank) then with 10 x $10^{-5}$Mof Simvastatin at room temperature for one day (24 h). Then, after this immersion time, the specimens were washed gently with distilled water, carefully dried and take carefully to the system of surface examinations such as using scanning electron microscope (SEM), energy dispersive x-ray (EDX) and atomic force microscope (AFM).

## III. Result and Discussion

*a) Potentiodynamic polarization technique*

Study the polarization of the different medium and with added the various concentration of Simvastatin as a corrosion inhibitor.

i. *Dissolution of LCH sample in 0.5 $NH_2SO_4$ at different temperatures*

Results of the anodic and cathodic polarization processes for the LCH sample in 0.5N $H_2SO_4$ at different temperatures in absence of Simvastatin are shown in Figure 2 and Table 2. It obvious that the corrosion current density ($I_{corr}$) is increased as the temperature

increased and the corrosion potential ($E_{corr}$) is slightly shafted to more positive value. The polarization processes are started with potential between of about 547 and 553 mV.

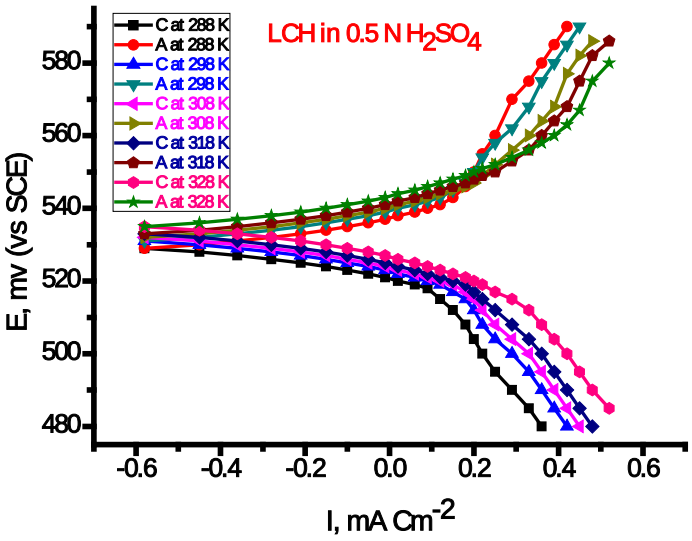



*Figure 2:* The potentiodynamic polarization curves for corrosion of LCH in 0.5 N of $H_2SO_4$

The positive potential is increased by anodic polarization, i.e. increase the dissolved component while that the potential decreased by cathodic polarization, i.e, increase the undissolved components. The dissolved component is formed as[29]:

$$Fe \rightarrow Fe^{2+} + 2e$$

$$Fe^{2+} + 2H_2O \rightarrow HFeO^-_2 + 3H^+$$

Where, $HFeO^-_2$ Di-hypo-ferrite, green.
In the same time occurs as:

$$HFeO_2^- + H^+ \rightarrow Fe(OH)_2$$

Where, the undissolved hydrated and the (FeO) can be considered. So that at anodic polarization in presence of $H_2SO_4$, the iron is dissolved and formed ferrous sulphate as:

$$Fe^{2+} + H_2SO_{4(aq)} \rightarrow Fe\,SO_{4(aq)} + 2H^+$$

And the cathodic processes in presence of $H_2SO_4$, occurred as:

i. $2H^+ + 2e \rightarrow H_2$ hydrogen evolution
ii. $O_{2(g)} + 4H^+_{(aq)} + 4e \rightarrow 2H_2O_{(l}$ reduced of oxygen

The hydrogen ions adsorbed on the metal surface where an electrochemical reaction takes place in presence of $O_2$ as;

$$M + H_3O^+ + e \rightarrow M{-}H + H_2O$$

Where three steps can be done as;

*a)* $2M{-}H \rightarrow 2M + H_{2(g)}\uparrow$
*b)* $M{-}H + H_3O^+ + e \rightarrow M + H_{2(g)}\uparrow + H_2O$ or
*c)* $4M{-}H^+ + \text{dissolved } O_2 + 4e \rightarrow 4M + 2H_2O_{(l)}$

ii. *Dissolution of LCH samples in 10% ethanol at various temperatures[30]*

Results of the anodic and cathodic polarization processes for LCH in 10 % ethanol at different temperatures in absence of Simvastatin is shown in Figure 3 and Table 2. It obvious that the corrosion current density ($I_{corr}$) is increased as the temperature increased and the corrosion potential ($E_{corr}$) is shafted to value that is more positive. The polarization processes are started with potential between of about 278 and 388 mV.

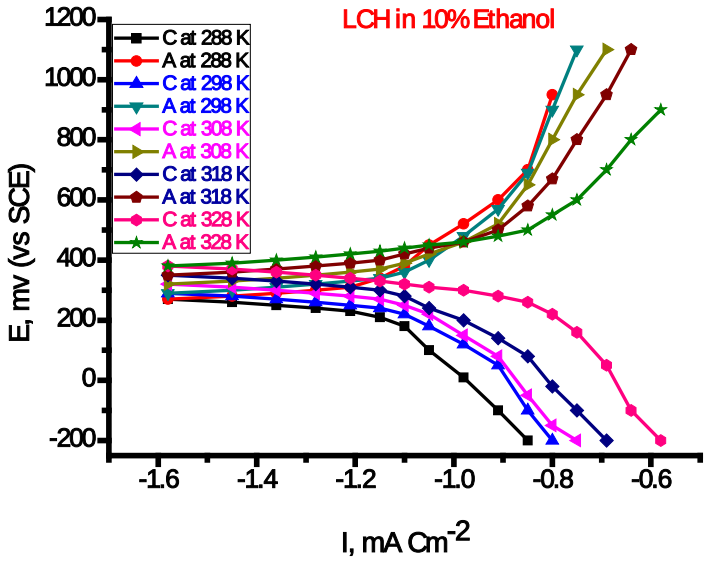



*Figure 3:* The potentiodynamic polarization curves for corrosion of (LCH) in 10% of ethanol

The positive potential is increased by anodic polarization, i.e. increase the dissolved component while that the potential decreased by cathodic polarization, i.e., increase the undissolved components. According to the following equation:

$$Fe \rightarrow Fe^{2+} + 2e \quad \text{anodic reaction}$$

$$2H_2O + 2e \rightarrow H_{2\,(g)}\uparrow + 2OH^- \quad \text{cathodic reaction}$$

In total process:

$$Fe + H_2O \rightarrow Fe^{2+} + 2OH^- \rightarrow Fe(OH)_2$$

In the bulk the ferrous hydroxide dissolved as:

$$2Fe(OH)_2 \rightarrow 2FeOH^{++} + 2OH^-$$

And, $2Fe\,OH^{++} + 2e \rightarrow 2Fe\,O + H_2\uparrow$

*Table 2:* The corrosion potential, corrosion current density and rate of corrosion for (LCH) in 10% ethanol and 0.5 N $H_2SO_4$ at various temperatures

| Concentration | Temp. | $E_{corr}$(mV) | $I_{Corr}$(mA/Cm$^2$) | Rate (mpy) |
|---|---|---|---|---|
| 10% Ethanol | 288K | 278 | 0.08 | 0.034 |
| | 298K | 298 | 0.09 | 0.038 |
| | 308K | 328 | 0.11 | 0.047 |
| | 318K | 358 | 0.12 | 0.051 |
| | 328K | 388 | 0.15 | 0.064 |
| 0.5 N $H_2SO_4$ | 288K | 547 | 5.46 | 2.33 |
| | 298K | 549 | 5.53 | 2.36 |
| | 308K | 550 | 5.65 | 2.41 |
| | 318K | 551 | 5.75 | 2.45 |
| | 328K | 553 | 5.90 | 2.51 |

iii. *Dissolution of LCH in mixed 0.5N $H_2SO_4$and 10%Ethanol (10A5H)*

Results of the anodic and cathodic polarization processes for (LCH) in mixed solution at different temperatures in absence of Simvastatin is shown in Figure 4 and Table 7. It obvious that the corrosion current density ($I_{corr}$) is increased as the temperature increased and the corrosion potential ($E_{corr}$) is shafted to the value that is more positive. The polarization processes are started with potential between of about 538 and 543 mV.

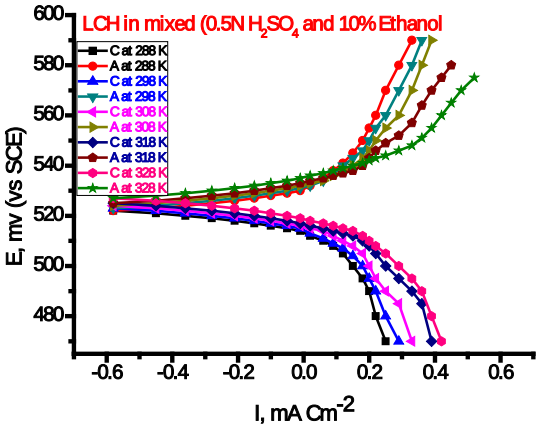



*Figure 4:* The potentiodynamic polarization curves for the corrosion of LCH in mixed [10A5H] in the nonexistence various concentration of Simvastatin at different temperatures

The positive potential is increased by anodic polarization, i.e. increase the dissolved component while that the potential decreased by cathodic polarization, i.e, increase the undissolved components. The results at 288K from Figure 5 and the comparison of $I_{corr}$ in those three media are listed in Table 3.

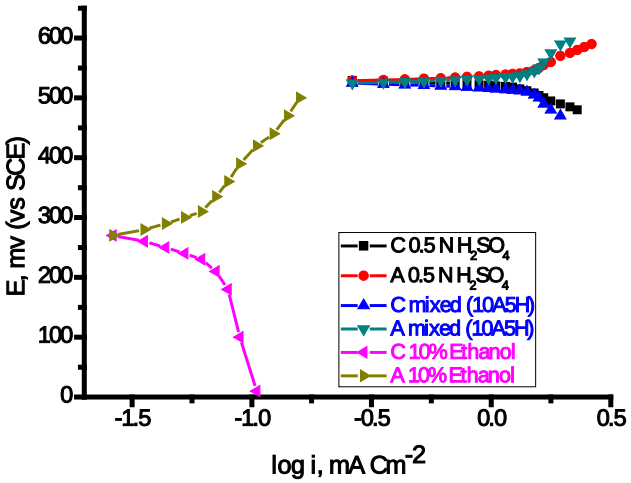



*Figure 5:* The comparison between the polarization effects in the three mediums of LCH at 288K

*Table 3:* Comparison between three medium

| Corrosive medium | Current density ($I_{corr}$) |
|---|---|
| | LCH |
| 10% Ethanol | 0.08 |
| 0.5 N $H_2SO_4$ | 5.46 |
| Mixed | 4.50 |

These results concluded that:

1- The corrosion rate in 0.5N $H_2SO_4$ is very high where the major product is the dissolved component $FeSO_4$ while the formation of undissolved component FeO is very low and slightly detected, where $I_{corr}$ is rise too (5.46)
2- In the second passivity region (in presence of 10% ethanol), the undissolved component is considered where the $I_{corr}$ is dropped to (0.08).
3- In the presence of mixed medium, the corrosion rate still very high where $I_{corr}$ is listed (4.50) and the undissolved component can be slightly considered.

iv. *Effect of 10% ethanol on the corrosion of steel in 0.5N $H_2SO_4$ at different temperature*

Result of the anodic and cathodic polarization of LCH in 0.5N $H_2SO_4$ with 10 % ethanol at different temperatures (288, 298, 308, 318 and 328K) are shown in Figure 4.

a. *Ptentiodynamic polarization technique*

In general, as the added 10% ethanol is shifted the potentials to less positive values comparing with only 0.5N $H_2SO_4$ and both anodic potential $E_a$ and cathodic potential $E_c$ are shifted to less positive values. The anodic current ($i_a$) slightly decreased (shifted to less values) while the cathodic ($i_c$) decreased and shifted to

less values too, Figures 6 at different temperatures. Values of corrosion potential ($E_{corr}$), corrosion current density ($I_{corr}$) and rate of corrosion in (mpy), are given in Table 7.

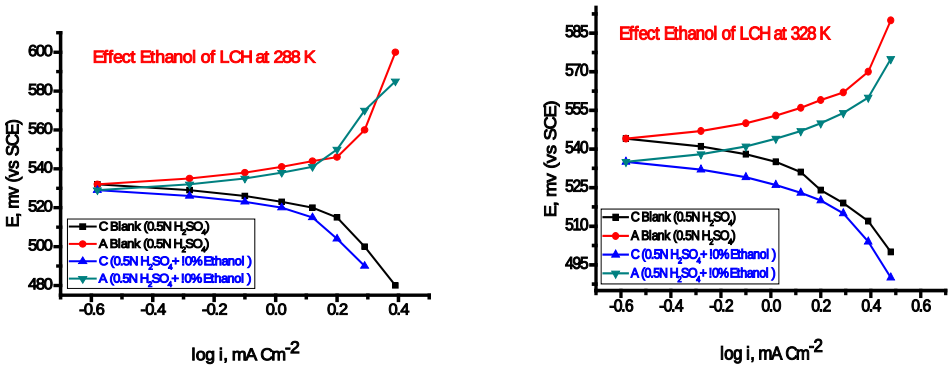



*Figure 6:* Effect of add 10% ethanol to 0.5N $H_2SO_4$ on anodic and cathodic polarization curves of LCH metal at various temperatures

b. *Applied Evans technique*

Applying the principle of Evans diagrams in presence of 10%ethanol with 0.5N $H_2SO_4$, was drown in Figures7 and the Evans diagram parameters was recorded in the Table4, it is clear that[31]:

The relative corrosion potential ($\Delta\phi_{corr}$) shifted slightly to more positive values. The relative corrosion current ($i_{corr}$) increases with temperatures increasing.

The potential difference ($\Delta\phi'_m$) is slightly increased with temperature increased and the potential difference ($\Delta\phi'_s$) is increased to high values too. The transference coefficient of cathode ($\alpha_c$) is slightly increased with temperature increasing but ($\alpha_a$) is slightly decreased with temperatures.

The anodic-potential difference $|\Delta\phi'_a|$ is not clear affect by temperature increased and the cathodic-potential difference $|\Delta\phi'_c|$ is slightly increased by temperature increased. The difference in anodic corrosion current $|\Delta I_a|$ is increased with temperature increased and the difference in cathodic corrosion current $|\Delta I_c|$ is slightly increased by temperature increased. The values of ratio ($\Delta\phi'_a/\Delta I_a$) are decreased by temperature increased and the values of ratio ($\Delta\phi'_c/\Delta I_c$) are decreased by temperature increased.

From the results illustrated in Evans diagrams for the electrode- electrolyte interface in (LCH) it is clear that:

The presence of 10% ethanol under polarization technique shifted the de-electronation potential toward more positive values (positive direction), this means that the polarization oriented and collective the ethanol molecules to the electron sink site on the electrode surface and slow down the metal dissolution. Moreover the presence of 10%ethanol under polarization technique shifted the electronation potential of acceptor spices to less positive values (negative directions), this means that the collective ethanol molecules are not only adsorbed on the electron sink area, but also the collective ethanol molecules covered the electron source area too. It is clear that, it slowing down (more and more) both the metal dissolution and the hydrogen evolution.

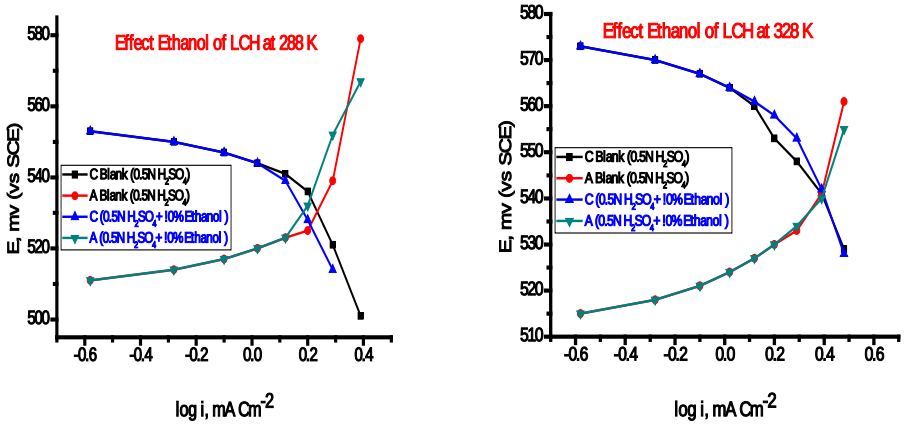



*Figure 7:* Evans diagrams of electronation and de-electronation potentials vs. log I for LCH in (10A5H) at various temperatures

*Table 4:* Relative parameters from Evans diagram of LCH in mixed solutions (10A5H).

| Temp. | Δφcorr | Icorr | Δφe,m | Δφe,so | Δφ'm | Δφ's | (i)b | (Δφ)b | (Δφ'a)x | Δφ'a | (Δla)x | Δla* | Δφ'a/Δlα | (Δφ'c)x | Δφ'c | (Δlc)x | Δlc | Δφ'c/Δlc | αa | αc |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 288 | 532 | 1.19 | 505 | 545 | 27 | 13 | 1.507 | 525 | 534 | 9 | 1.21 | 0.3 | 30.1 | 519 | 6 | 1.39 | 0.12 | 51.28 | 0.68 | 0.33 |
| 298 | 533 | 1.3 | 503 | 549 | 30 | 16 | 1.585 | 527 | 535 | 8 | 1.32 | 0.3 | 29.96 | 520 | 7 | 1.48 | 0.11 | 66.04 | 0.65 | 0.35 |
| 308 | 539 | 1.41 | 501 | 553 | 38 | 14 | 1.66 | 528 | 537 | 9 | 1.41 | 0.2 | 36.44 | 526 | 2 | 1.62 | 0.04 | 52.63 | 0.73 | 0.27 |
| 318 | 540 | 1.52 | 501 | 555 | 39 | 15 | 1.95 | 532 | 541 | 9 | 1.51 | 0.4 | 20.64 | 526 | 6 | 1.74 | 0.21 | 28.3 | 0.72 | 0.28 |
| 328 | 541 | 1.59 | 500 | 560 | 41 | 19 | 2.344 | 537 | 543 | 6 | 1.66 | 0.7 | 8.772 | 526 | 11 | 1.95 | 0.39 | 27.92 | 0.68 | 0.32 |

v. *Effect of add different concentration of Simvastatin inhibitor*

Result of the anodic and cathodic polarization of LCH in mixed solution (10A5H) with different concentrations of Simvastatin(2, 4, 6, 8 and 10x10$^{-5}$ M) at 288K are shown in Figure 8.

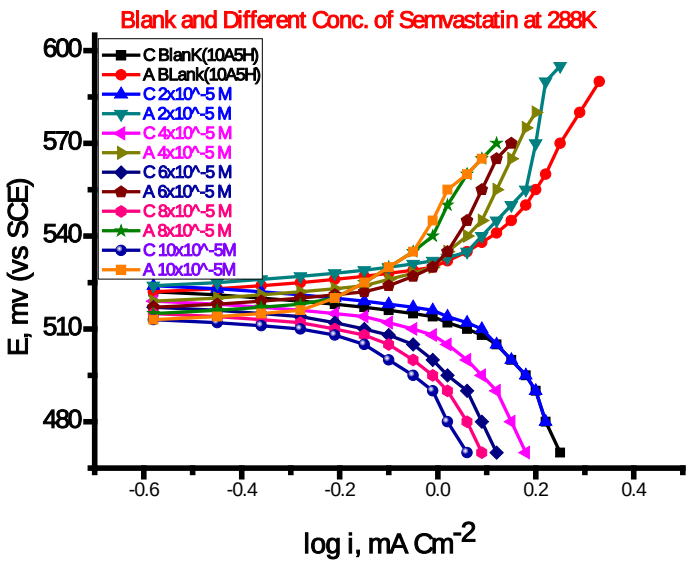



*Figure 8:* The potentiodynamic polarization curves for the corrosion of LCH in 10A5H with existence various concentration of Simvastatin at 288K

a. *Potentiodynamic polarization technique*

It is obvious that the presence of different concentrations are shifted the potentials to less positive values and both anodic potential $E_a$ and cathodic potential $E_c$ are shifted to less positive values. The anodic current ($i_a$) slightly decreased (shifted to less values) while the cathodic ($i_c$) decreased and shifted to less values too shown in Figure 9.

Values of corrosion potential ($E_{corr}$), corrosion current density ($I_{corr}$) and rate of corrosion in (mpy), are given in Table 7.

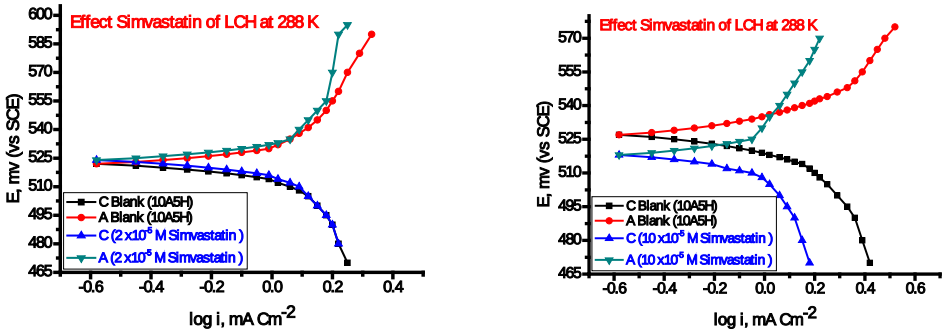



*Figure 9:* Effect of add different concentration of Simvastatinon anodic and cathodic polarization curves of LCH metal at constant temperature 288K

b. *Applying Evans technique*

Applying the principle of Evans diagrams in presence of different concentrations from Simvastatin, which are viewed in Figures 10, and the Evans diagram parameters are listed in Table 5, it is clear that:

The relative corrosion potential ($\Delta\phi_{corr}$) shifted slightly to less positive values. The relative corrosion current ($i_{corr}$) decreases with temperatures increasing.

The potential difference ($\Delta\phi'_m$) is decreased with temperature increased and the potential ($\Delta\phi'_s$) is increased to high values by increasing temperatures. The transference coefficient of cathode ($\alpha_c$) is increased with temperature increasing but the transference coefficient of anode ($\alpha_a$) is decreased with temperatures increased.

The anodic-potential difference $|\Delta\phi'_a|$ is increased by temperature increased and the cathodic-potential difference $|\Delta\phi'_c|$ is increased by temperature increased. The difference in anodic corrosion current $|\Delta I_a|$ is increased with temperature increased and the difference in cathodic corrosion current $|\Delta I_c|$ is increased by temperature increased. The values of ratio ($\Delta\phi'_a/\Delta I_a$) are decreased by temperature increased and the values of ratio ($\Delta\phi'_c/\Delta I_c$) are decreased by temperature increased.

From the results illustrated in Evans diagrams for the electrode- electrolyte interface in both (LCH), it is clear that:

In presence concentrations of Simvastatin under polarization technique, at low Simvastatin concentrations the de-electronation potential shifted toward more positive values (positive direction) this means that the polarization affected the donor functional groups of Simvastatin molecules and oriented them to the electron sink area on the electrode surface and slow done the dissolution of metal. The moderate size of Simvastatin molecules allow to cover some what area of electron source, so that the electronation potential of acceptor spices to less positive value. It is observed that the shifted of de-electronation potential is larger than the shift of electronation potential. As the Simvastatin concentration increased the shift of electronation potential i.e, the Simvastatin molecules covered more electron source area on the corroded metal surface with increasing Simvastatin concentration and the electronation potential shift is being larger than the de-electronation potential shift, which indicates slightly formation of multilayer that adsorbed on the electrode surface. It is clear that the polarization process affects the orientation and adsorption of the inhibitor molecules, so that both the metal dissolution and the hydrogen evolution is slowing down more.

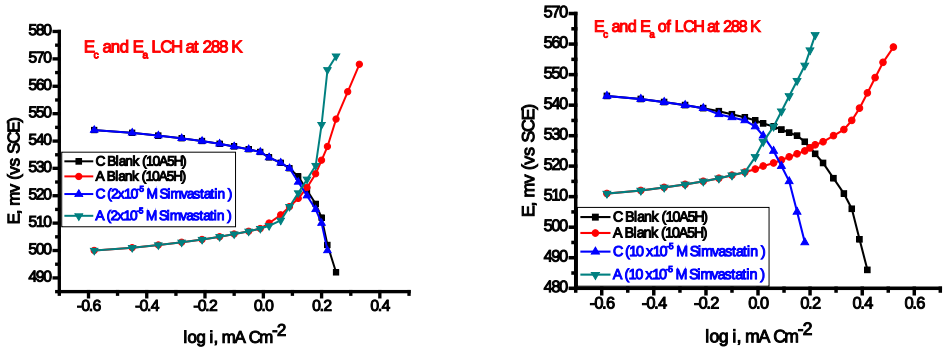



*Figure 10:* Evans diagrams of electronation and de-electronation potentials vs log I for LCH with various concentration of Simvastatin at 288K

*Table 5:* Relative parameters from Evans diagram of LCH with various concentration of Simvastatin at 288K

| Temp. | Δφcorr | Icorr | Δφe,m | Δφe,so | Δφ'm | Δφ's | (i)b | (Δφ)b | (Δφ'a)x | Δφ'a | (Δla)x | Δla* | Δφ/Δl,a | (Δφ'c)x | Δφ'c | (Δlc)x | Δlc | Δφ'/Δl,c | α,a | α,c |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 288 | 526 | 1.38 | 499 | 547 | 27 | 21 | 1.514 | 523 | 528 | 5 | 1.41 | 0.1 | 49.5 | 521 | 2 | 1.48 | 0.03 | 57.14 | 0.56 | 0.44 |
| 298 | 525 | 1.29 | 499 | 547 | 26 | 22 | 1.514 | 523 | 530 | 7 | 1.35 | 0.2 | 42.42 | 518 | 5 | 1.38 | 0.13 | 37.31 | 0.54 | 0.46 |
| 308 | 524 | 1.18 | 499 | 547 | 25 | 23 | 1.514 | 523 | 533 | 10 | 1.26 | 0.3 | 39.22 | 514 | 9 | 1.27 | 0.24 | 37.5 | 0.52 | 0.48 |
| 318 | 523 | 1.05 | 499 | 547 | 24 | 24 | 1.514 | 523 | 535 | 12 | 1.12 | 0.4 | 30.61 | 512 | 11 | 1.23 | 0.28 | 38.73 | 0.5 | 0.5 |
| 328 | 522 | 1 | 499 | 547 | 23 | 25 | 1.514 | 523 | 536 | 13 | 1.1 | 0.4 | 31.1 | 510 | 13 | 1.18 | 0.34 | 38.35 | 0.48 | 0.52 |

vi. *Effect of temperature on corrosion behavior*

Results of the anodic and cathodic polarization processes for the LCH sample in corrosive medium. The $E_{corr}$, $I_{corr}$ and the rate of corrosion were increased with temperatures increased at the same concentration ($4x10^{-5}$M) of Simvastatin, which are listed in Table 7 and Figure 11.

a. *Potentiodynamic polarization technique*

This behavior indicating to the corrosion rate of LCH stimulates with increasing of temperature and increasing of temperatures will be enhance the rate of diffusion of hydrogen ($H^+$) ion to the metal surface beside the ionic mobility, thus increasing the conductivity of the electrolyte. Also, at lower temperatures, absorbed hydrogen atoms which are blocked on the cathodic areas, otherwise the increasing temperatures of the solution, hydrogen will be disrobed, from the cathodic area, i.e the corrosion rate increased.

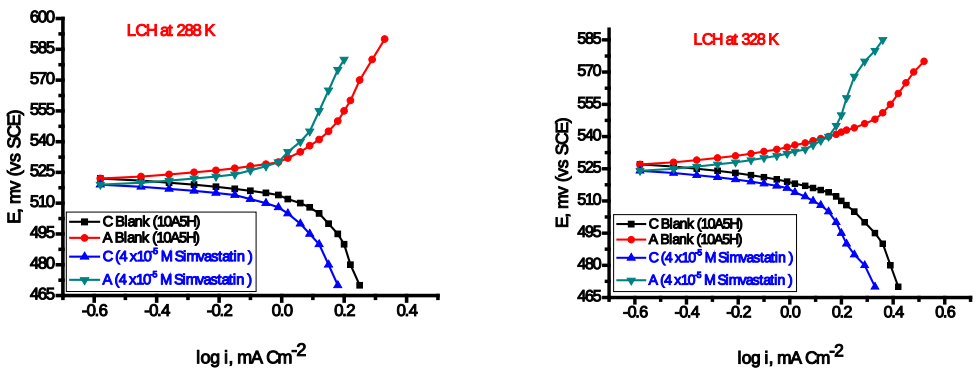



*Figure 11:* Effect of temperatures in presence $4x10^{-5}$M of Simvastatin on anodic and cathodic polarization curves of LCH metal

a. *Apply Evans technique*

Applying the principle of Evans diagrams in presence of $4x10^{-5}$M from Simvastatin, which are viewed in Figures 12 and the Evans diagram parameters are listed in Table 6, it is clear that: The relative corrosion potential ($\Delta\phi_{corr}$) shifted slightly to less positive values. The relative corrosion current ($i_{corr}$) increases with temperatures increasing.

The potential difference ($\Delta\phi'_m$) is slightly decreased with temperature increased and the the potential ($\Delta\phi'_s$) is increased to high values by increasing temperatures. The transference coefficient of cathode ($\alpha_c$) is increased with temperature increasing but the transference coefficient of anode ($\alpha_a$) is decreased with temperatures increased.

The anodic-potential difference $|\Delta\phi'_a|$ is increased by temperature increased and the cathodic-potential difference $|\Delta\phi'_c|$ is decreased by temperature increased. The difference in anodic corrosion current $|\Delta l_a|$ is increased with temperature increased and the difference in cathodic corrosion current $|\Delta l_c|$ is increased by temperature increased. The values of ratio

$(\Delta\phi'_a/\Delta I_a)$ are decreased by temperature increased and the values of ratio $(\Delta\phi'_c/\Delta I_c)$ are decreased by temperature increased.

From the results illustrated in Evans diagrams for the electrode- electrolyte interface it is clear that:

The effect of temperature on the behavior of Simvastatin as inhibitor of LCH corrosion, at $4x10^{-5}$M Simvastatin. It obvious that both electronation and de-electronation potentials are shifted to negative and positive direction respectively by increasing the temperature. This behavior clarify that the heat treatment (quenching) divided the electron sink and electron source area to small parts, so that the size of Simvastatin sufficient to cover more electron source area be side electron sink.

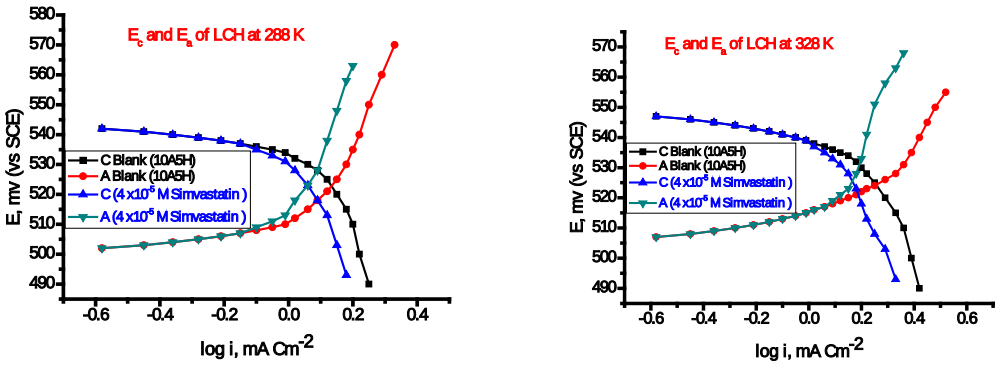



*Figure 12:* Evans diagrams of electronation and de-electronation potentials vs. log I for LCH in presence of $4x10^{-5}$M of Simvastatin at various temperatures

*Table 6:* Relative parameters from Evans diagram of LCH in presence of $4x10^{-5}$M of Simvastatin at various temperatures

| | Δφcorr | Icorr | Δφe,m | Δφe,so | Δφ'm | Δφ's | (i)b | (Δφ')b | (Δφ'a)x | Δφ'a | (Δla)x | Δla* | Δφ/ | (Δφ'c)x | Δφ'c | (Δlc)x | Δlc | Δφ'/ | α,a | α,c |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 288 | 528 | 1.19 | 500 | 544 | 28 | 16 | 1.413 | 528 | 530 | 2 | 1.26 | 0.2 | 12.99 | 518 | 10 | 1.29 | 0.13 | 80 | 0.64 | 0.36 |
| 298 | 525 | 1.29 | 499 | 547 | 26 | 22 | 1.514 | 524 | 531 | 7 | 1.35 | 0.2 | 42.42 | 517 | 7 | 1.38 | 0.13 | 52.24 | 0.54 | 0.46 |
| 308 | 524 | 1.35 | 498 | 550 | 26 | 26 | 1.66 | 524 | 534 | 10 | 1.41 | 0.2 | 40.49 | 516 | 8 | 1.48 | 0.18 | 44.2 | 0.5 | 0.5 |
| 318 | 528 | 1.48 | 497 | 553 | 31 | 25 | 1.95 | 524 | 537 | 13 | 1.59 | 0.4 | 35.62 | 517 | 7 | 1.62 | 0.33 | 21.34 | 0.55 | 0.45 |
| 328 | 526 | 1.62 | 497 | 557 | 29 | 31 | 2.291 | 521 | 536 | 15 | 1.74 | 0.6 | 27.12 | 515 | 6 | 1.89 | 0.4 | 14.93 | 0.48 | 0.52 |

*Table 7:* The effect of (Simvastatin) additions on the $E_{corr}$, $I_{corr}$ and rate of corrosion for (LCH) in (10A5H) at various temperatures

| Conc.[I]x $10^5_M$ | Temp. K | $E_{corr}$ (mV) | $I_{corr}$ ($mA/Cm^2$) | Rate (mpy) | Θ | % IE |
|---|---|---|---|---|---|---|
| 0.00 | 288 | 538 | 4.50 | 1.92 | ---- | ---- |
| | 298 | 539 | 4.60 | 1.96 | ---- | ---- |
| | 308 | 540 | 4.82 | 2.06 | ---- | ---- |
| | 318 | 541 | 4.95 | 2.11 | ---- | ---- |
| | 328 | 543 | 5.20 | 2.28 | ---- | ---- |
| 2.00 | 288 | 537 | 1.31 | 0.56 | 0.709 | 70.9 |
| | 298 | 538 | 1.35 | 0.58 | 0.706 | 70.6 |
| | 308 | 539 | 1.41 | 0.60 | 0.707 | 70.7 |
| | 318 | 541 | 1.48 | 0.63 | 0.700 | 70.0 |
| | 328 | 543 | 1.60 | 0.68 | 0.702 | 70.2 |
| 4.00 | 288 | 535 | 1.27 | 0.54 | 0.718 | 71.8 |
| | 298 | 536 | 1.31 | 0.56 | 0.715 | 71.5 |
| | 308 | 537 | 1.39 | 0.59 | 0.712 | 71.2 |
| | 318 | 538 | 1.44 | 0.61 | 0.709 | 70.9 |
| | 328 | 539 | 1.54 | 0.65 | 0.712 | 71.2 |
| 6.00 | 288 | 533 | 1.24 | 0.53 | 0.724 | 72.4 |
| | 298 | 534 | 1.28 | 0.55 | 0.722 | 72.2 |
| | 308 | 535 | 1.35 | 0.58 | 0.720 | 72.0 |
| | 318 | 536 | 1.41 | 0.60 | 0.715 | 71.5 |
| | 328 | 537 | 1.46 | 0.62 | 0.727 | 72.7 |
| 8.00 | 288 | 531 | 1.21 | 0.51 | 0.731 | 73.1 |
| | 298 | 532 | 1.26 | 0.54 | 0.726 | 72.6 |
| | 308 | 533 | 1.32 | 0.56 | 0.726 | 72.6 |
| | 318 | 534 | 1.37 | 0.58 | 0.723 | 72.3 |
| | 328 | 535 | 1.42 | 0.61 | 0.735 | 73.5 |
| 10.00 | 288 | 529 | 1.191 | 0.51 | 0.735 | 73.5 |
| | 298 | 530 | 1.22 | 0.52 | 0.735 | 73.5 |
| | 308 | 531 | 1.27 | 0.54 | 0.737 | 73.7 |
| | 318 | 532 | 1.33 | 0.57 | 0.732 | 73.2 |
| | 328 | 533 | 1.40 | 0.60 | 0.738 | 73.8 |

*b) Inhibition efficiency (IE %)*

The Simvastatin compound has eight active centers as; oxygen atoms an π-bonding act as donor center. Because of the restricted un-plainer structure of Simvastatin, not all active group acts in the same time. These centers orientedand adsorbed to anodic sites (iron carbide). The Simvastatin molecule attached with anodic site and covered somewhat of cathodic area, so that the corrosion rate in presence of Simvastatin is anodic-cathodic control. The inhibition efficiency (IE %) is calculated as following [32].

$$IE\ \% = [(I_{corr} - I'_{corr})/I_{corr}] \times 100 \quad (1)$$

Where; $I_{corr}$ and $I_{corr}'$ are the corrosion current density in absence and presence of inhibitor respectively. The inhibition efficiency data in Table7, obvious that this inhibition efficiency for LCH sample under study increases with increasing Simvastatin concentration in the following order:

$$10^{-4} > 8x10^{-5} > 6x10^{-5} > 4x10^{-5} > 2x10^{-5}\ M$$

Plot IE % against logarithm of Simvastatin inhibitor (log [I]), obvious that in cases 288, 298, 308 and 318K the inhibition efficiency (IE %) decreased as the temperature of the medium is increased, but the (IE %) in 328K increased, this behavior indicated that chemisorption's occurs. See Figure13. The extra part in the curvatures that obtained from polarization technique than S shape indicates that there are multilayer proceed from the orientation of functional group under polarization where caused second chemical adsorption over the first layer[33].

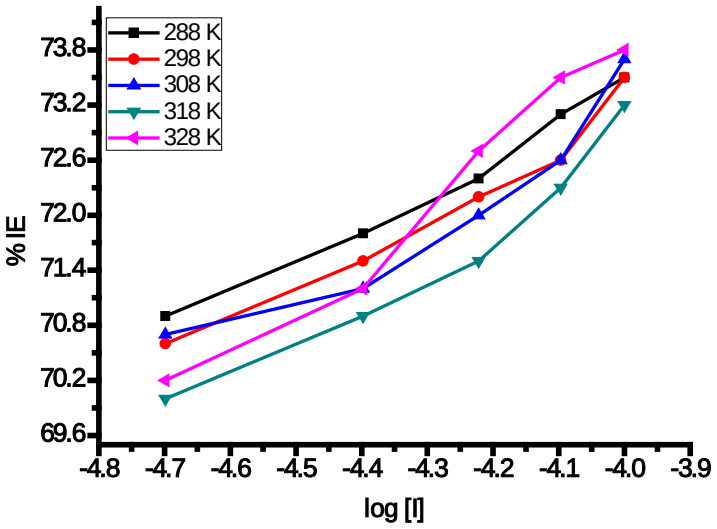
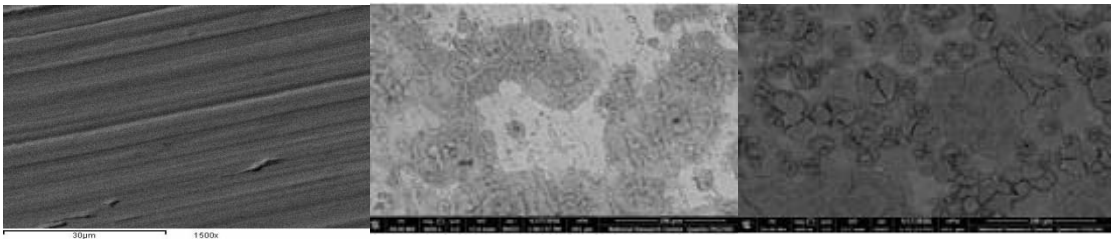



*Figure 13:* The relation between inhibition efficiency and log [I] in (10A5H) for LCH at various temperatures

c) *Scanning Electron Microscopy (SEM)*

The micrographs that obtained for LCH specimens in nonexistence and in existence of 10 x $10^{-5}$M of Simvastatin drug after exposure forimmersion one day in corrosive medium(10A5H). It is clear that LCH is suitable surfaces for corrosion attack in the blank sample or in corrosive medium only Figures 14 a, b and c. When the Simvastatin is existence in the corrosive medium, the morphology of LCH surfaces is quite different from the previous one, and the specimen surface was smoother. It is clear that the formation of a thin layer film adsorbed on the metal surface, which distributed in a disorder way overall surface of the LCH. This may be due to the adsorption of the Simvastatin on the LCH surface and made up the passive film in order to block the active site present on the LCH surface. The Simvastatin molecule interaction with active sites of LCH surface, resulting in a decrease in the contact between LCH and the corrosive medium and sequentially exhibited excellent inhibition effect[34].



a-Free sample (LCH) b- Blank in (10A5H) 10 x $10^{-5}$M of Simvastatin c-In (10A5H) with existence

*Figures 14 a, b and c:* SEM micrographs for LCH in the nonexistence and existence of 10 x $10^{-5}$M of Simvastatin after submersion for 1 day

d) *Energy Dispersion Spectroscopy (EDX)[35]*

To determination the elements and molecules that existence or adsorbed on the surface of MS after one day that immersion in acid with optimum doses of Simvastatin by using the EDX spectra. Figure 15, gives the EDX analysis of LCH in (10A5H) with in the presence of 10 x $10^{-5}$M of Simvastatin. The spectra show additional lines, demonstrating the existence of C (owing to the carbon atoms of some Simvastatin). These data shows that the carbon, nitrogen and oxygen atoms covered the specimen surface. The EDX analysis indicates that only nitrogen, carbon and oxygen are detect and show that the passivation film contained the chemical formula of Simvastatin drag adsorbed on the surface of LCH. It is clear that, the percent weight of adsorbed elements C and O were present in the spectra and recorded in (Table 8).

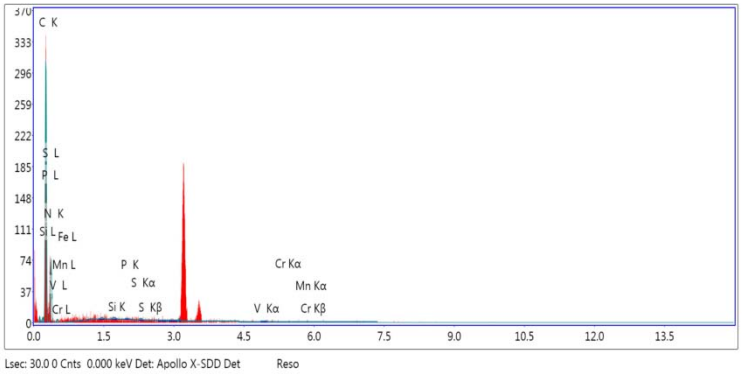


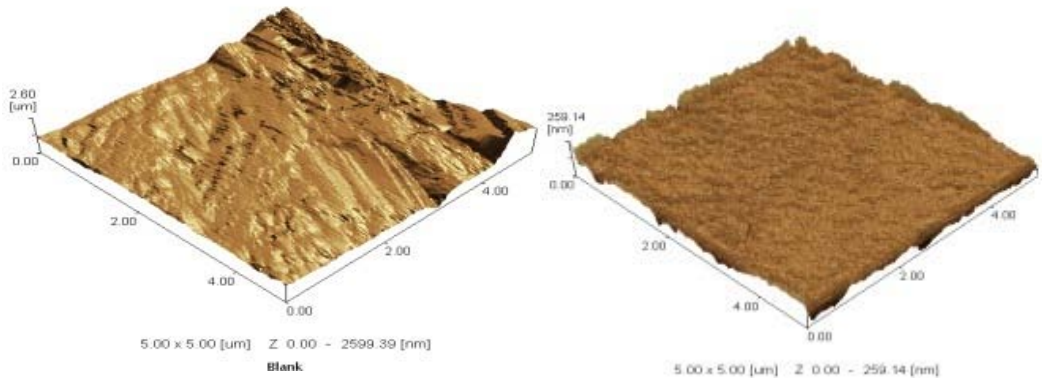

*Figure 15:* EDS analysis on LCHin the existence10 x $10^{-5}$M Simvastatin drug for 1 day immersion in (10A5H)

*Table 8:* Surface composition (wt %) of LCHafter one day of immersion in (10A5H) without and with the 10 x $10^{-5}$M of Simvastatin

| (wt %) | Fe | C | O | N | S | Cl |
|---|---|---|---|---|---|---|
| Simvastatin | 62.16 | 1.32 | 33.54 | 1.14 | -- | 1.63 |

*e) Atomic Force Microscopy (AFM)*

AFM is a powerful tool to investigate the surface morphology of various samples at nano- micro scale that is currently used to study the influence of corrosion inhibitors on metal solution interface. From the analysis, it can be gained regarding the roughness on the surface. The roughness profile values play an important role in identifying and report the efficiency of the inhibitor under study. Among the roughness, take a role in explanation about the nature of the adsorbed film on the surface [36-37]. Figure 16a, shows the 3D images as well as elevation profiles of polished of LCH in absence and present Simvastatin as an inhibitor. It observed in Figure 16b, the surface of LCH specimen (a) exposed to corroded solution affected vales structure with large and deep crack but the surface (b) reveal that is covering film adsorbed on the metal surface. The conclusion, that the adsorption film can protect the surface of the metal from corrosion process. Analysis of the values indicated higher the values of roughness parameter reached. The mean roughness is found to be (2.60 $\mu$m) for the blank in acid solution which placed in (10A5H) one day and analyzed. The observation of the metal surface which immersed in (10A5H) in presence of 10 x $10^{-5}$Mof Simvastatin inhibitor possess roughness (259.14 nm) compared to the blank solution. It can be noted that the value is lower than that of the blank value. The decrease in the roughness value reflected to the adsorption of inhibitor molecule on metal surface thereby reducing the rate of corrosion.




a-Blank b-In presence 10 x $10^{-5}$M of Simvastatin drug

*Figure 16 a and b:* The 3D of optical images of AFM in nonexistence and existence of Simvastatin drug

*f) Mechanism of inhibition*

To illustrate the mechanism of inhibition of corrosion on the LCH surface in acid medium by using pharmaceutical drug compound as an inhibitor, it is must be know the nature of metal surface and the nature of the component of inhibitor structure. The LCH is regarded the metal α-phase[38], It is obvious that α-phase state consists of grains and grain boundaries in the surface of the metal, Figure 17. A cross-section of a piece or specimen of the metal that is a corroding to clarify that there are both anodic and cathodic sites in the metal surface structure.

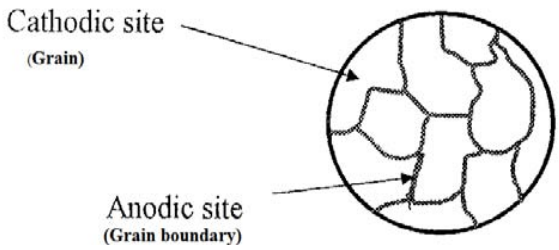



*Figure 17:* Schema models of metalα- phase

The surface of iron is usually, coated with a thin film of iron oxide. However, if this iron oxide film develops some cracks, anodic area are created on the surface, while other metal parts act as cathodes. It follows that the anodic areas are small surface, while nearly the rest of the surface of the metal large cathodes. Electrochemical corrosion involves flow of electric current between the anodic and cathodic areas called inter-granular corrosion Figure 18. SEM image is shown the corrosion of LCH in 0.5 N $H_2SO_4$in one day immersion that illustrated inter-granular corrosion.

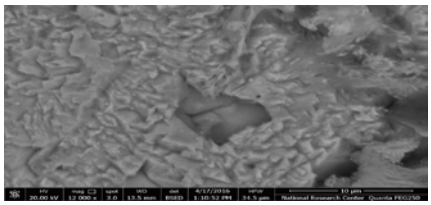


*Figure 18:* SEM image illustrated inter-granular corrosion after immersion the specimen in 0.5N $H_2SO_4$one day

All previous results prove that the pharmaceutical drug compound under study were actually inhibit the corrosion of LCH in $H_2SO_4$ acid solution as a corrosive medium. The corrosion inhibition is due to their physical adsorption and formation of protection thin film adsorbed on the metal surface.The effect of Simvastatin as inhibitor may be corresponding to the accumulation of the inhibitor molecules on the metal surface, which prevent the direction contact of the metal surface with corrosive environment. The surface of the LCH sample is positively charge in aqueous acid solution and the adsorption occur according to[39-40]:

1. The partial negative charge that present in function group containing Oxygen and electron density of π-bond in Simvastatin may be adsorbed on the positively charge of the metal surface like electrostatic attraction between the opposite charge, in the form of neutral molecules, that involving displacement of water molecules from the metal surface.
2. The unshared electrons of oxygen atomsand electron density of π bondingdonate to the vacant orbital on the metal surface like chemisorption[41].
3. The inhibition action of the inhibitor can be accounted by the interaction between the lone pair of electrons in the O and electron density of π-bond with positively charged (anodic sites) on the metal surface and the skeleton of inhibitor compound cover the cathodic sites this action form thin layer adsorbed on the metal surface and prevent corrosion processes Figure 19.

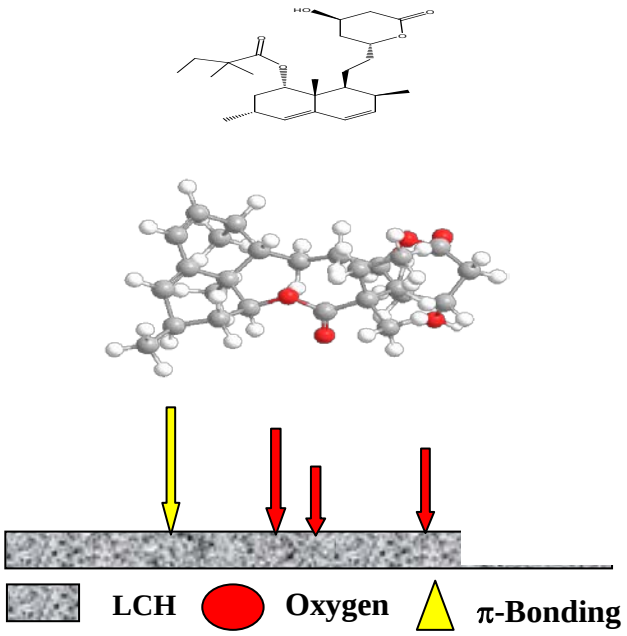



*Figure 19:* Schema model illustrated the adsorption of Simvastatinstructure on the (LCH) surface

This meaning, the Simvastatin molecule attached with anodic site and covered somewhat of cathodic area, so that the corrosion rate in presence of Simvastatin is anodic-cathodic control.

## IV. Conclusion

Inhibition of the corrosion of LCH in (10A5H) solution by Simvastatin is determine by potentiodynamic polarization and Evans techniques and surface examination by Scanning Electron Microscopy (SEM), energy Dispersive X-ray (EDX) and atomic force microscopy (AFM). It was found that the inhibition efficiency depends on concentration, nature of metal surface, the type of adsorption of the inhibitor. The observed corrosion data in presence Simvastatin inhibitor, namely:

1) The tested Simvastatininhibitor establish a very good inhibition for LCH corrosion in 10A5H solution
2) Simvastatininhibit the LCH for the corrosion by adsorption on its surface and make thin film layer.
3) The inhibition efficiencies of the tested compound increase with increasing of their concentrations.
4) The values of inhibition efficiencies obtained from the two techniques used, showed the validity of the obtained results.

5) The Simvastatinmolecule attached with anodic site and covered somewhat of cathodic area, so that the corrosion rate in presence of Simvastatinis anodic-cathodic control.

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# Chemopreventive Action of Compounds from *Parmelia Perlata*

By Sonal Dobhal, Maheep Kumar, Yogesh Chandra Joshi & Ashok Kumar

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*Keywords:* *Cancer, Parmelia Perlata, Ethanolic Extract, LPO, SOD.*

*GJSFR-B Classification:* *FOR Code: 030199*


*Strictly as per the compliance and regulations of:*

# Chemopreventive Action of Compounds from *Parmelia Perlata*

Sonal Dobhal [α], Maheep Kumar [σ], Yogesh Chandra Joshi [ρ] & Ashok Kumar [ω]

*Abstract-* Cancer prevention may be accomplished by phytochemicals obtained from vegetables, fruits, spices, teas, herbs and medicinal plants. The investigations on the species of *Parmelia* proved to be source of unique chemical agents that have already been proved to be effective against various types of cancer. Present study focus on chemopreventive activity against random-bred male *Swiss albino* mice through oral administration of dried ethanolic extract of traditional medicinal lichen *Parmelia perlata*. Further ethanolic extract of entitled lichen afforded three novel compounds.

*Keywords: Cancer, Parmelia Perlata, Ethanolic Extract, LPO, SOD.*

## I. Introduction

Cancer is classes of disease in which cells do not follow the defined programmed growth pattern rather divided in random uncontrolled manner to invade surrounding tissues and metastasize. Some of the major known reasons behind cancer are- spreadness of western diets, increasing tobacco consumption, relentless industrialization, chemicals, radiation, infectious organisms and internal factors like inherited mutations, hormones and immune status. All reasons lead to serious derangement of the ecosystem such that cancer has emerged as a deadly disease across the globe. However, it is now clear that the cause of cancer is not due to one single event, but a multi-factorial phenomenon. These risk factors either together or in sequence can initiate or promote carcinogenesis [1].

There is an urgent need to develop mechanism-based approaches for the management of cancer i.e. to develop strategies, which can eliminate only the damaged or malignant cells without harming the normal ones. Basically cancer chemoprevention mechanism uses natural, synthetic or biochemical agents to inhibit the development of invasive cancer by either blocking the DNA damage or by arresting or reversing the progression of premalignant cells [2]. In recent years, natural products have been emerged as one of major route of cancer chemotherapy because of its diverse pharmacological properties [3]. However, the prompt pace of gene identification and the new technologies of combinatorial chemistry, high-throughput screening, should provide access to a wide range of totally newly synthetic drugs. Natural products are likely to provide several lead structures and used as templates for the construction of novel compounds with enhanced biological properties.

*Parmelia perlata* (Lichen) belonging to faimily Parmeliaceae is one of the potent anticancerous agent. It is commonly known as "Charila" in India and mostly found in hilly region. It is a lichen composed mainly of fungal mycelia that forms a network where algal cells or gonidia are enclosed. It grows in rosettes or spread irregularly over the substratum and resembles a flower in its appearance. Three lichen acids- namely, (+)-usnic acid, vulpinic acid and atranorin were isolated from *Parmelia tinctorum* showed *in vitro* antioxidant effects on mice-liver mitochondrial [4]. Extracts of *Parmelia caperata* demonstrated interesting activities particularly on human cancer cell lines [5]. Gyrophoric, usnic, and diffractaic acid have been shown antiproliferative and cytotoxic activity on human keratinocyte growth [6].

The objective of our study was to explore lichen, *Parmelia perlata* as a chemopreventive agent. Its efficacy has been examined against 7, 12-Dimethylbenzene ($a$) anthracene (DMBA) and croton oil induced skin papillomas. In our study, mouse skin model of two stage carcinogenesis has been taken as the experimental protocol for various reasons. One of the merit is the latent period which is relatively short in the case of tumours, and therefore, expanse of time for observation is not too long. Animals are not sacrificed for the tumours, as they are externally visible and hence can be scored easily. Also, they are non lethal and efficacy of compound as a potential chemopreventive agent can be concluded by having a look at the number of tumors on the skin of the animal.

## II. Results

In group I (control) all the animals were treated with Dimethylbenzene ($a$) anthracene (DMBA) that was applied once topically and later on after two weeks promoter (croton oil) was applied. Skin papillomas were visible on almost all the animals (100 ± 0.00 percent).

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Animals treated orally in the group II, group III, group IV and group V with the extract of *Parmelia perlata* showed significant reduction(66.66 ± 3.33, 76.66 ±3.33, 73.33 ± 3.33 and 56.66 ± 3.33 respectively) ($p<0.001$) in the tumor incidence i.e. percent as compared to control group which is calculated to be 100±0.00 percent [Table 1 and Graph 1]. The average number of tumors per tumor bearing mouse (Tumor burden) was (3.11 ± 0.34, 3.22 ± 0.13, 2.63 ± 0.31, 1.73 ± 0.17 respectively) that was significantly lessen comparison to control group (4.63 ± 0.08) [Table 2 and Graph 2]. Increase in average latent period was observed i.e. 11 ± 0.57, 13.66 ± 0.33, 12 ± 0.00, 14 ± 0.00 respectively as compared to control group (11.66 ± 0.66) [Table 3 and Graph 3].

*a) Biochemical studies*

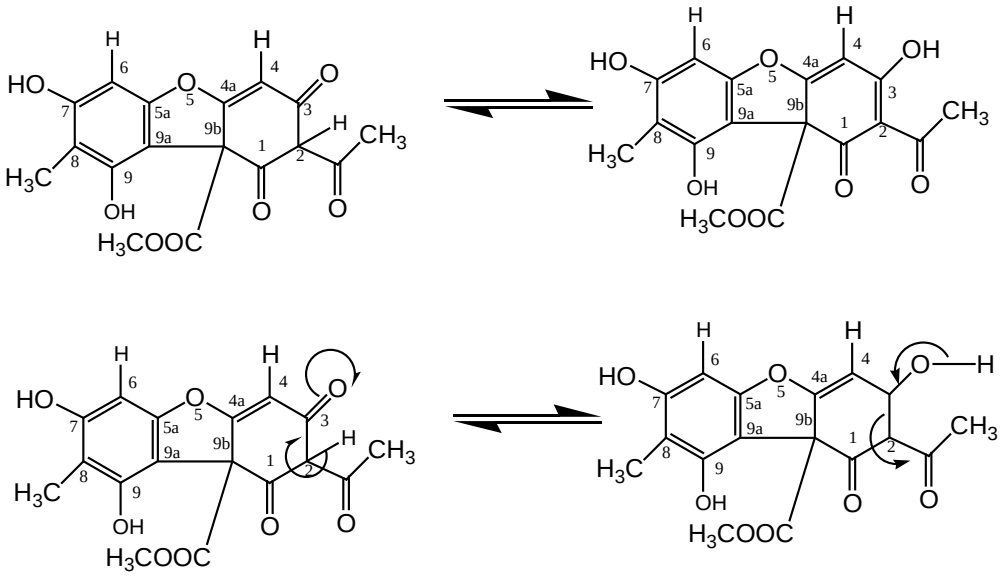
The Glutathione (GSH) value of animals of control group was 2.31 ± 0.12, but the animals that were treated with ethanolic extract at pre initiational stage reported 3.05 ± 0.06 ($p<0.01$) value, for peri initiational stage it was 3.06 ± 0.06 ($p<0.01$), 3.71 ± 0.06 ($p<0.01$) was calculated for animals in post initiational stage and mice treated in throughout initiational stage showed i.e. 3.64 ± 0.07 ($p<0.001$), GSH values that are significantly high as compared to control group. All animals in control group showed high value for Lipid peroxidation (LPO) i.e. 9.00 ± 0.24, whereas animals of pre group showed low values ($p<0.001$) for LPO i.e. 6.09 ± 0.20, same with peri group mice with significantly low ($p<0.05$) LPO values (6.12 ± 0.59), significant decrease ($p<0.001$) in post initiational stage mice i.e. 6.04 ± 0.22, and 6.24 ± 0.44 ($p<0.01$) was observed for animals that were treated at throughout initiational stage [Table 4 and Graph 4].

*b) Compound obtained from ethanolic extract*

When the column was eluted with different solvents in order of increasing polarity following compounds were obtained.

i. *Isolation of compound 'A' as (+)-6-deacetyl-9b-carbmethoxy-9b-demethylusnic acid*

Compound 'A' was obtained when column was eluted with petroleum ether. After solvent removal, a yellow solid mass was obtained which on crystallization with ethyl acetate yielded shining yellow crystals. It showed single spot on TLC examination ($R_f$= 0.35) in petroleum ether: chloroform (3: 1). The melting point of this compound was found to be 131$^0$C. Compound 'A' in solution exists in two tautomeric forms i.e., ketonic and enolic [7-14].



**(+)-6-Deacetyl-9b-carbmethoxy-9b-demethylusnic acid**

*Structure 1*

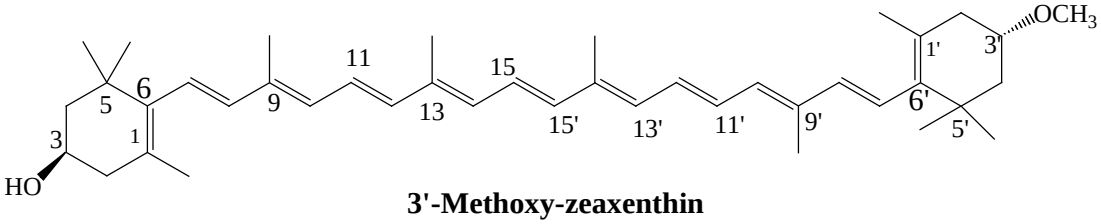
*c) Spectral data*

IR (KBr, cm$^{-1}$): 3410 (O-H stretching),1780 (>C=O, str.), 1555(>C=C< str.), 1055 (C-O, str.) etc.; $^1$H NMR (δ ppm, $CDCl_3$): 2.53 (s, 3H, C-2, -$COCH_3$), 5.13 (s, 1H, C-4, -H ), 6.47 ( s, 1H, C-6, -H), 13.32 ( s, 1H, C-7, -OH ), 2.18 (s, 3H, C-8, -$CH_3$), 11.98 ( s, 1H, C-9, -OH), 4.04 (s, 3H, C-9b, -$COOCH_3$),; $^{13}$C NMR (δ ppm, $CDCl_3$): 197.19 (C-1), 108.49 (C-2), 200.38 (-$COCH_3$ at C-2), 31.69(-$COCH_3$ at C-2), 166.65 (C-3), 101.58 ( C-4), 178.11(C-4a), 140.16 (C-5a), 99.13 (C-6), 165.11 (C-7), 108.49 (C-8), 7.69 (-$CH_3$ at C-8), 158.02(C-9), 105.18 (C-9a), 59.87(C-9b), 172.02 (-$COOCH_3$ at C-9b), 52.31(-

$COOCH_3$ at C-9b); MS (m/z): 346($M^+$), 347 ($M^+$ +H), 259, 232, 165 etc; Molecular formula: $C_{17}H_{14}O_8$ (Calculated).

i. *Isolation of compound 'B' as 3'-Methoxy-zeaxenthin*

It was isolated as intense orange-red crystalline compound when we eluted column with mixture of petroleum ether with chloroform (1:1) and it showed single spot on TLC examination. Melting point of compound was found to be 163 $^0$C [15].




**3'-Methoxy-zeaxenthin**

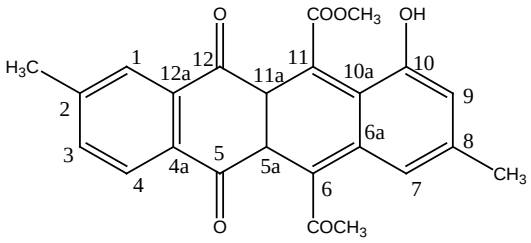
*Structure 2*

*d) Spectral data*

IR (KBr,$cm^{-1}$): 3410 (O-H stretching), 1440, 1370 (-$CHMe_2$ gem bend.) 1625(>C=C< str.), 1105 (C-O, str.) etc. $^1$H NMR (δ ppm, $CDCl_3$): 2.61 (s, 3H, C-3', -$OCH_3$), 5.13-6.00 (m, 1H, for 14 conjugated protons), 4.11( s, 1H, C-3, -OH ), 1.45-1.91 (m, 3H, for remaining 38 protons). $^{13}$C NMR (δ ppm, $CDCl_3$): 28.03 (C-5), 29.43 (C-1'), 45.31 (C-2), 49.24 (C-4), 50.68 (C-2'), 65.89(C-3), 75.38(C-3'), 42.01(C-4'), 140.90-143.07 (C-1, C-6, C-5' and C-6'), 132.01-134.01(Complicated pattern for conjugated carbon); MS (m/z): 580($M^+$), 581($M^+$ +H ), 565, 550, 535, 400, 364, 277, 212 etc.; Molecular formula(Calculated): $C_{41}H_{56}O_2$.

i. *Isolation of compound 'C' as 6-acetyl-11-carbmethoxy-10-hydro xy-2, 8-dimethylnaphthacene-5, 12-quinone (New)*

Compound 'C' was obtained when column was eluted with petroleum ether. After removal of solvent, it was redissolving in acetone. Acetone soluble part was crystallized into yellow shining crystals. It showed single spot on TLC examination in petroleum ether: chloroform (4:1) mixture. The melting point of this compound was found to be 141$^0$C.




**6-Acetyl-11-carbmethoxy-10-hydroxy-2,8-dimethyl nahthacene-5, 12-quinone**

*Structure 3*

*e) Spectral data*

IR (KBr, $cm^{-1}$): 3310 (O-H stretching) 1733, 1762 (>C=O, str.), 1625(>C=C< str.), 1053 (C-O, str.) etc. $^1$H NMR (δ ppm, $CDCl_3$): 2.52 (s, 3H, C-2, -$CH_3$), 6.47 (s, 1H, C-9), 2.77 ( s, 3H, C-6, -$COCH_3$), 2.11 (s, 3H, C-8, -$CH_3$), 12.41( s, 1H, C-10, -OH), 4.00 (s, 3H, C-11, -$COOCH_3$, 6.13(d, 1H, C-3), 6.29 (s, 1H, C-7), 6.22 (s, 1H, C-1), 6.17 (d, 1H, C-4). $^{13}$C NMR (δ ppm, $CDCl_3$): 162.09 (C-1), 109.21 (C-2), 10.25 (C-2, -$CH_3$), 110.49 (C-3), 161.09 (C-4), 115.75 (C-4a), 181.35 (C-5), 141.21(C-6), 194.10 ( -$COCH_3$ at C-6), 24.10( -$COCH_3$ at C-6), 108.21 (C-6a), 163.23 (C-7), 137.21 (C-8), 28.21 ($CH_3$ at C-8), 118.14 (C-10), 128.51 (C-11), 178.25(-$COOCH_3$ at C-11), 51.79 (-$COOCH_3$ at C-11), 187.23 (C-12), 153.44 (C-11a); MS (m/z): 402($M^+$), 403 ($M^+$ +H), 401, 385 etc; Molecular formula(Calculated): $C_{24}H_{18}O_6$.

## III. Discussion

The study conducted on *Parmelia perlata* signifies that the oral administration of the vacuum dried ethanolic extract of *Parmelia perlata* at pre, peri, post and throughout initiational phases showed a significant reduction in tumor incidence, tumor burden, and a significant increase in average latent period and displayed a significant increase in GSH whereas a significant decrease was observed for LPO. The chemopreventive effects of the natural dietary compounds includes antioxidative, anti-inflammatory

activity, induction of phase I and phase II enzymes, apoptosis and cell cycle arrest. Recently, attention has been focused on intracellular-signalling cascades as common molecular targets for various chemopreventive natural dietary compounds [16]. Data obtained after epidemiological and experimental studies provided the information that antioxidants also includes a vast variety of nutritional factors in inhibiting or reducing the risk of cancer. Such antioxidants include vitamin A, C and E, beta carotene, and micronutrients [17].

Lichens have been found to contain a variety of secondary lichen substances and have attracted the attention of investigators for over 100 years. The most known lichen substances are usnic acid, phenolic compounds, anthraquinones, dibenzofurans, depsides, depsidones, depsones, triterpenes, gamma lactones and pulvinic acid derivatives and exhibit multiple biological activities such as antiviral, antibiotic, antitumor, allergenic, plant growth inhibitory and enzyme inhibitory [18]. Usnic and atranorin acids like secondary metabolites were found out to be effective in the suppression of viability and cell proliferation at equitoxic doses and also demonstrated increased number of floating cells or a higher apoptotic index [19].

Therefore, because of the presence of secondary metabolites in the lichens, they have immune-modulating properties, potent antibiotic, antitumor, antiviral as well as antioxidant properties [20]. Further, the ethanolic extract was observed for its reduced glutathione level. GSH act as an antioxidant, as by reacting with singlet oxygen, hydroxyl radicals and superoxide it can function as a free radical scavenger. Also, by removing acyl peroxides formed as a result of lipid peroxidation, GSH may stabilize membrane structure [21]. Moreover, study reported GSH acts as a reducing agent by recycling ascorbic acid (vitamin C) from its oxidized form to its reduced form by dehydroascorbate reductase enzyme [22]. The enhanced levels of Glutathione prevents the oxidation of cellular proteins and detoxifies reactive oxygen species directly. Oxygen free radicals play an important role in stimulating cancer development al all three stages of carcinogenesis i.e. initiation, promotion and progression [23]. The increased reduced glutathione level plays a significant role in the reduction of oxidized glutathione to reduced glutathione at the expenses of NADPH and regulates GSH-GSSG cycle in the cell [24]. Hence, glutathione is often considered as the first line of defense against oxidative stress. Also, the elevated levels of GSH protects proteins in the cells against oxidation through redox cycle and detoxifies reactive oxygen species directly and/or neutralizes reactive intermediate species generated from exposure to xenobiotics including chemical carcinogens [25]. Membranes where the unsaturated fatty acids content is relatively high, lipid peroxidation occurs. Free radicals are fundamentals to any biochemical processes and represent an essential part of aerobic life and metabolism. It may be defined as any species, that is capable of independent existence and contains one or more unpaired electrons. Free radicals are atoms or groups of atoms with at least one unpaired electron and because of this they are highly reactive. They are highly toxic in nature and if accumulated they can destroy macromolecules like lipids, proteins, mitochondrial and nuclear DNA molecules of the cells and causes oxidative stress [26]. To safeguard against the fatal effects of free radicals and their derivatives all cells and tissues of our body are equipped with antioxidative enzymes like superoxide dismutase (SOD), glutathione peroxidase (GPx), glutathione reductase (GR) and substances like glutathione (GSH), they dispose the free radicals as and when they are generated thereby protecting the cells and tissues from the oxidative attack. About 1-4% of oxygen taken up in the body is converted as free radicals.

Increase in the activity of Chloramphenicol acetyltransferase (CAT) enhances the free radical scavenging activity of SOD. At the present time, it is suspected that lichens do act as potent antioxidants, therefore, in search for new natural antioxidant sources, attention has been focused on lichens [27]. Lichens produce secondary metabolites like depsides, depsidones, dibenzofurans and phenolic compounds, and they possess biological activities like antimicrobial, antipyretic, antiproliferative, cytotoxic, antitumor, analgesic and antioxidant [28]. In the laboratory it was revealed that lichens behaves as antioxidant because of presence of particular types of compounds [29]. The investigations on the species of Parmelia proved to be source of unique chemical agents that have already been proved to be effective against various cancers. Among these few reported compounds some showed activity against few human cancers [6].

Usnic acid and atranorin are effective anti-cancer compounds, they both have the capability to induce a massive loss in the mitochondrial membrane potential, along with activation of Caspase3 (only in HT-29 cells) and phosphatidylserine externalization in both tested cell lines. It was observed that both usnic acid and atranorin are activators of programmed cell death in A2780 and HT-29 through mitochondrial pathway [30]. Usnic acid may be considered for non-genotoxic anticancer drugs, as it without causing any DNA damage to DNA can decrease the proliferation of human breast cancer cells and human lung cancer cells [31].

## IV. Materials and Methods

*Animal:* Random-bred male Swiss albino mice (7-8 weeks age old) were maintained in the animal house at temperature of 24˚±3˚C and at light of 14:10 hours of light and dark. The animals housed in polypropylene

cages and were fed standard feed. Tap water was provided and tetracycline was given monthly to the animals against infections.

*a) Chemicals*

DMBA and croton oil will be obtained from Sigma Chemicals Co., USA., Dithio-bis-2-nitrobenzoic acid (DTNB), 2-thiobarbituric acid (TBA), the ethanolic extract of titled plant was considered for the biological activity.

*Parmelia perlata* after collection were dried in shade. The shade dried plant material was grinded to make powder and was extracted with different organic solvents (petroleum ether, chloroform, ethyl acetate and ethanol). On elucidation three novel compounds viz. (+)-6-deacetyl-9b-carbmethoxy-9b-demethylusnic acid, 3'-Methoxy-zeaxenthin and 6-acetyl-11-carbmethoxy-10-hydroxy-2,8-dimethyl naphtha- acene-5,12-quinone along with known compounds.

i. *Experimental Design*

Three days before the commencement of the experiment, the dorsal skin of the animals in the interscapular area was shaved and the resting phase of hair cycle of animals were studied. For the experimental protocol, the two stage mouse skin carcinogenesis model was selected. A single topical application of carcinogen DMBA was used for induction of tumour (100 µg/50µl acetone per animal). Initiation, DMBA was followed by the application of the promoter (croton oil) three times a week (100 µl on dorsal surface of each animal) (10µl per ml acetone).

To see the effects of *Parmelia perlata* on DMBA/croton oil induced skin papillomagenesis the experiment was designed in which animals were divided into five groups and were treated separately. They were marked and weighed prior the experiment and were shaved before treatment for the better distribution of the chemical.

Total of 45 animals for Group II, III, IV, V and VI were randomly divided into the following five groups. Three days before the commencement of the experiment, the dorsal skin of the animals in the inters capulararea were clipped. Only the mice in the resting phase of the hair cycle were considered for the study. In 16 weeks of experiment, mice were observed and weighed weekly. Mice were carefully examined and recorded once a week.

*Group I: (n=9)*

Animals were treated with DMBA (100 µg/50µl acetone per animal). 100µl of croton oil was applied on the shaven area after two weeks, and was continued three times in a week for 14 weeks.

*Group II: (n=9)*

Animals were treated with *Parmelia perlata* extract for 7 days before application of DMBA. After two weeks croton oil was applied and was continued three times in a week for 14 weeks.

*Group III: (n=9)*

Animals were treated with *Parmelia perlata* extract 14 days after the application of DMBA. Two weeks after DMBA application croton oil was applied and continued three times in a week for 14 weeks.

*Group IV: (n=9)*

Animals were treated with DMBA and two weeks after DMBA application croton oil was applied and was continued three times in a week for 14 weeks. *Parmelia perlata* extract was given to animals from the day of croton oil application till the end of the experiment (three times a week).

*Group V: (n=9)*

Animals were treated with *Parmelia perlata* extract before 7 days of DMBA application and the treatment of *Parmelia perlata* extract was continued throughout the experiment (16 weeks). Two weeks after DMBA application croton oil was applied and was continued three times in a week for 14 weeks.

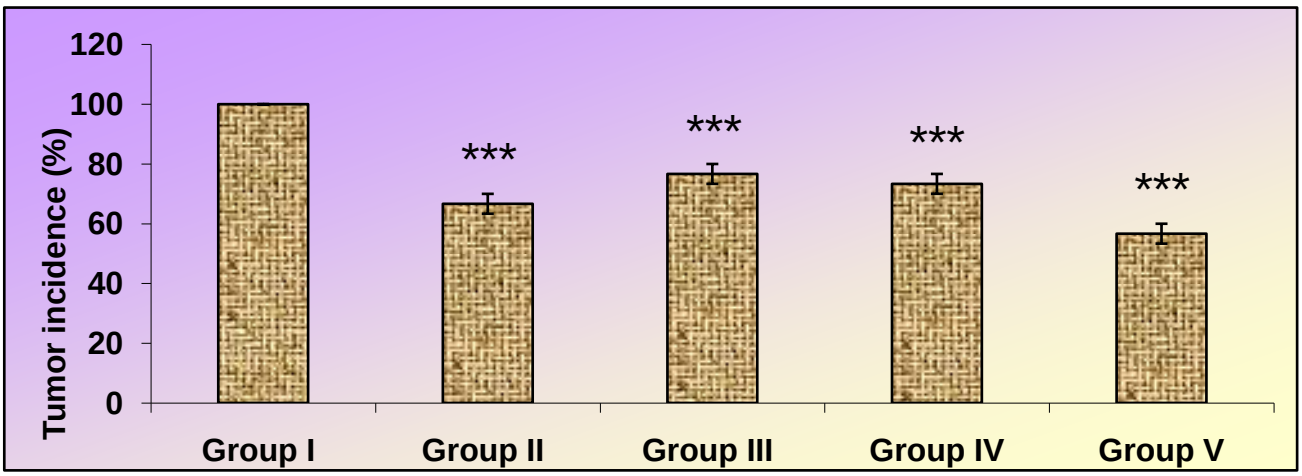
*b) Tumor study*

The following morphological parameters were studied in groups I-V:

1. *Tumor incidence:* The number of mice carrying at least one tumor expressed as a percentage incidence (Table 1 and Graph 1).

*Table 1:* Tumor incidence recorded after initiation by DMBA, followed by 2 weeks later by croton oil treatment (three times a week) for 14 weeks with or without treatment of *Parmelia perlata* (800 mg/kg body weight/day)

| Group | Treatment | Drug Duration | Tumor incidence (%) | Remarks |
|---|---|---|---|---|
| Group I | DMBA (100 μg/50 μ l acetone) + Croton oil (100 μg of 1% conc.) | - | 100±0.00 | CONTROL 16 weeks duration |
| Group II | DMBA (100 μg/50 μl acetone + Croton oil (100 μg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 7 days | 66.66±3.33*** | *Parmelia perlata* (800 mg/kg body wt./day) at pre initiational stages of papillomagenesis |
| Group III | DMBA (100 μg/50 μl acetone+Croton oil (100 μg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 14 days | 76.66±3.33*** | *Parmelia perlata* (800 mg/kg body wt./day) at periinitiational stages of papillomagenesis |
| Group IV | DMBA (100 μg/50 μl acetone+Croton oil (100 μg of 1% conc.) + *Parmelia perlata* (800 mg/kg body wt./day | 14 weeks | 73.33±3.33*** | *Parmelia perlata* (800 mg/kg body wt./day) at post initiational stages of papillomagenesis |
| Group V | DMBA (100 μg/50 μl acetone+Croton oil (100 μg of 1% conc.) + *Parmelia perlata* (800 mg/kg body wt./day | 14 weeks | 56.66±3.33*** | *Parmelia perlata* (800 mg/kg body wt./day) at pre, peri, post initiational stages of papillomagenesis |



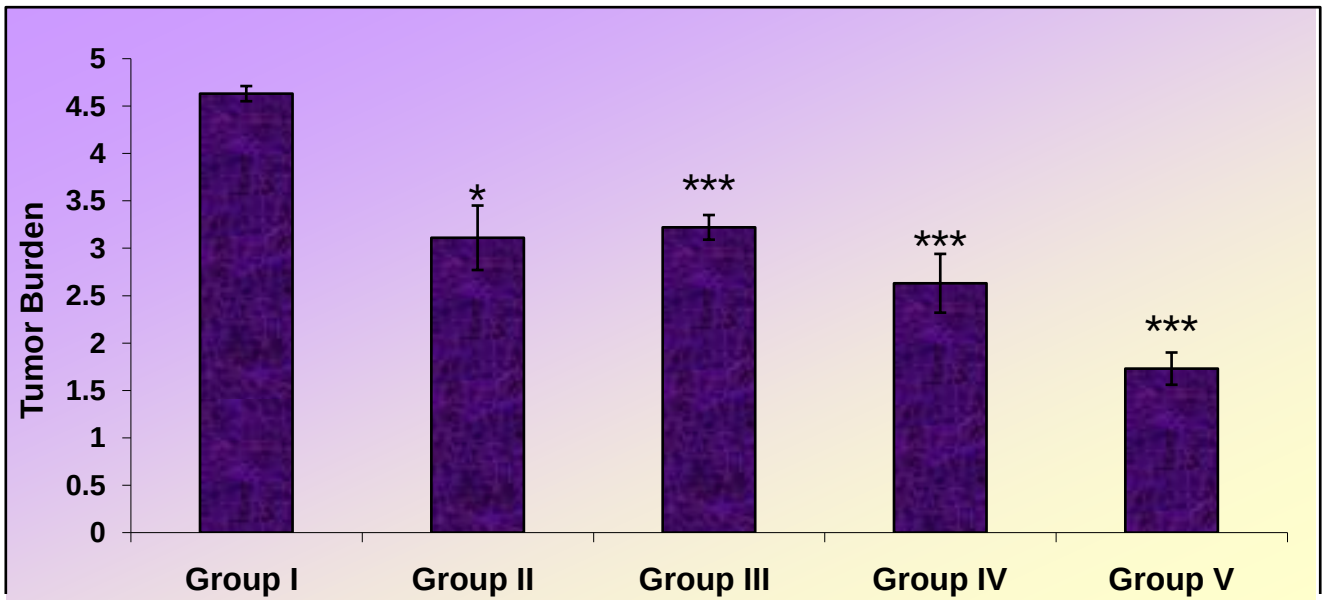

Group I: CONTOL- 16 weeks duration
Group II: Pre-initiational stage (800mg/kg body wt./day)
Group III: Peri-initiational stage (800mg/kg body wt./day)
Group IV: Post-initiational stage (800mg/kg body wt./day)
Group V: Throughout-initiational stage (800mg/kg body wt./day)

*Graph 1:* Tumor incidence recorded after initiation by DMBA, followed by 2 weeks later by croton oil treatment (three times a week) for 14 weeks with or without treatment of *Parmelia perlata* (800 mg/kg body weight/day)

2. *Tumor burden:* The average number of tumors per tumor bearing mouse (Table 2 and Graph 2).

*Table 2:* Tumor burden observed after initiation of DMBA, followed 2 weeks later by croton oil treatment (three times in a week) for 14 weeks with or without treatment for *Parmelia perlata* (800 mg/kg b. wt./day).

| Group | Treatment and Dose | Drug Duration | Tumor Burden | Remarks |
|---|---|---|---|---|
| Group I | DMBA (100 μg/50 μ l acetone) + Croton oil (100 μg of 1% conc.) | - | 4.63±0.08 | CONTROL 16 weeks duration |
| Group II | DMBA (100 μg/50 μl acetone + Croton oil (100 μg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 7 days | 3.11±0.34* | *Parmelia perlata* (800 mg/kg body wt./day) at pre initiational stages of papillomagenesis |
| Group III | DMBA (100 μg/50 μl acetone + Croton oil (100 μg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 14 days | 3.22±0.13*** | *Parmelia perlata* (800 mg/kg body wt./day) at periinitiational stages of papillomagenesis |
| Group IV | DMBA (100 μg/50 μl acetone + Croton oil (100 μg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 14 weeks | 2.63±0.31*** | *Parmelia perlata* (800 mg/kg body wt./day) at pre, peri, post initiational stages of papillomagenesis |
| Group V | DMBA (100 μg/50 μl acetone + Croton oil (100 μg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 14 weeks | 1.73±0.17*** | *Parmelia perlata*(800 mg/kg body wt./day) at pre, peri, post initiational stages of papillomagenesis |




Group I: CONTOL- 16 weeks duration
Group II: Pre-initiational stage (800mg/kg body wt./day)
Group III: Peri-initiational stage (800mg/kg body wt./day)
Group IV: Post-initiational stage (800mg/kg body wt./day)
Group V: Throughout-initiational stage (800mg/kg body wt./day)

*Graph 2:* Tumor burden observed after initiation of DMBA, followed 2 weeks later by croton oil treatment (three times in a week) for 14 weeks with or without treatment for *Parmelia perlata* (800 mg/kg b. wt./day)

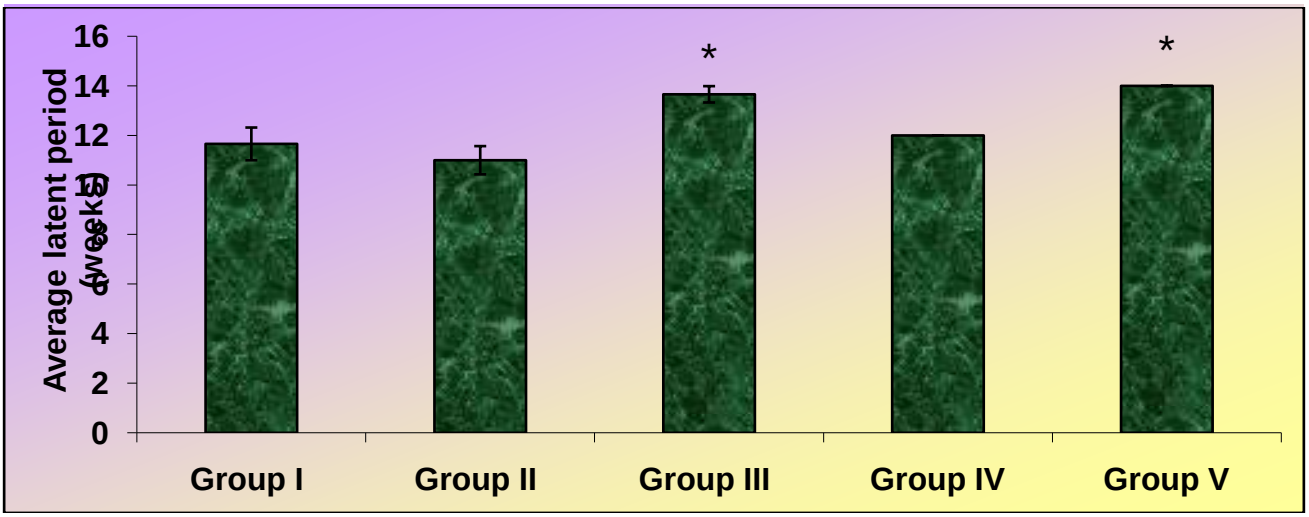
3. *Average latent period:* The time lag between the application of the promoting agent and the appearance of 50% of tumors was determined. The average latent period was calculated by multiplying the number of tumors appearing each week after the application of the promoting agent and dividing the sum by total number of tumors (Table 3 and Graph 3).

Average latent period= SFX/n

Where, F is the number of tumors appearing in each week, X is the number of weeks and n is the total number of tumors.

*Table 3:* Average latent period observed afterinitiation of DMBA, followed 2 weeks later by croton oil treatment (three times in a week) for 14 weeks with or without treatment for *Parmelia perlata* (800 mg/kg b. wt./day).

| Group | Treatment and Dose | Drug Duration | Average Latent period (weeks) | Remarks |
|---|---|---|---|---|
| Group I | DMBA (100 μg/50 μ l acetone) + Croton oil (100 μg of 1% conc.) | - | 11.66±0.66 | CONTROL 16 weeks duration |
| Group II | DMBA (100 μg/50 μl acetone + Croton oil (100 μg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 7 days | 11±0.57 | *Parmelia perlata*(800 mg/kg body wt./day) at pre, initiational stages of papillomagenesis |
| Group III | DMBA (100 μg/50 μl acetone + Croton oil (100 μg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 14 days | 13.66±0.33* | *Parmelia perlata* (800 mg/kg body wt./day) at peri, initiational stages of papillomagenesis |
| Group IV | DMBA (100 μg/50 μl acetone + Croton oil (100 μg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 14 weeks | 12±0.00 | *Parmelia perlata* (800 mg/kg body wt./day) at post initiational stages of papillomagenesis |
| Group V | DMBA (100 μg/50 μl acetone + Croton oil (100 μg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 14 weeks | 14±0.00* | *Parmelia perlata* (800 mg/kg body wt./day) at peri, peri, post initiational stages of papillomagenesis |




Group I: CONTOL- 16 weeks duration

Group II: Pre-initiational stage (800mg/kg body wt./day)

Group III: Peri-initiational stage (800mg/kg body wt./day)

Group IV: Post-initiational stage (800mg/kg body wt./day)

Group V: Throughout-initiational stage (800mg/kg body wt./day)

*Graph 3:* Average latent period observed after initiation of DMBA, followed 2 weeks later by croton oil treatment (three times in a week) for 14 weeks with or without treatment for *Parmelia perlata* (800 mg/kg b. wt./day).

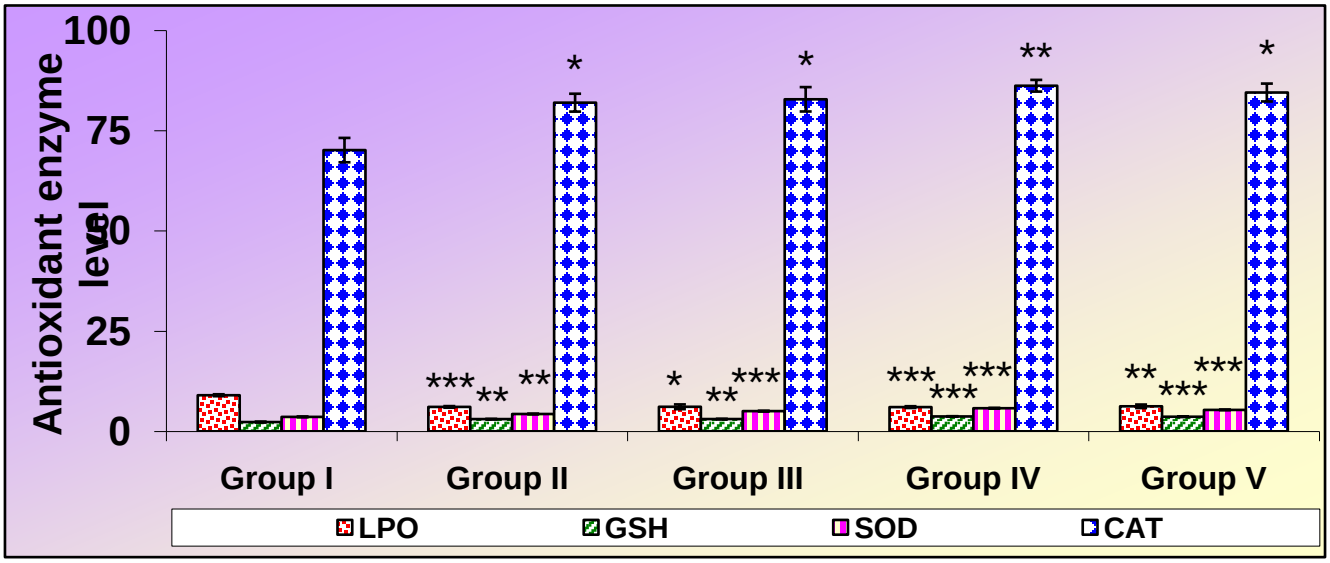
c) *Biochemical Study*

To study the reduced glutathione content and lipid peroxidation level in liver of *Swiss albino* mice the experiment was designed and the animals were grouped as follows (Table 4 and Graph 4):

*Table 4:* The modulatory effect of 800mg/kg b. wt./day of *Parmelia perlata* extract on the GSH, LPO, SOD and CAT levels in the tissue of *Swiss albino* mice after initiation of DMBA, followed 2 weeks later by croton oil treatment (three times in a week) for 14 weeks with or without treatment for *Parmelia perlata*

| Group | No.of animals | Treatment and Dose | Drug Duration | LPO (n mole/mg protein) | GSH (n mole/gm tissue) | SOD (μ mol/mg protein) | CAT (n mole/mg protein) | Remarks |
|---|---|---|---|---|---|---|---|---|
| Group I | 9 | DMBA (100 μg/50 μ l acetone) + Croton oil (100 μg of 1% conc.) | - | 9.0±0.24 | 2.31± 0.12 | 3.6± 0.10 | 70.14± 3.04 | CONTROL 16 weeks duration |
| Group II | 9 | DMBA (100 μg/50 μl acetone + Croton oil (100 μg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 7 days | 6.09± 0.2*** | 3.05± 0.06** | 4.32± 0.10** | 81.97± 2.23* | *Parmelia perlata* (800 mg/kg body wt./day) at peri, peri, post initiational stages of papillomagenesis |
| Group III | 9 | DMBA (100 μg/50 μl acetone + | 14 days | 6.12 ±0.59* | 3.06± 0.06** | 5.04± 0.10*** | 82.81± 3.04* | *Parmelia perlata*(800 mg/kg body wt./day) at |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | Croton oil (100 µg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | | | | | | peri, peri, post initiational stages of papillomagenesis |
| Group IV | 9 | DMBA (100 µg/50 µl acetone + Croton oil (100 µg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 14 weeks | 6.04± 0.22*** | 3.71± 0.06*** | 5.76± 0.10*** | 86.19± 1.46** | *Parmelia perlata* (800 mg/kg body wt./day) at post initiational stages of papillomagenesis |
| Group V | 9 | DMBA (100 µg/50 µl acetone + Croton oil (100 µg of 1% conc. + *Parmelia perlata* (800 mg/kg body wt./day | 14 weeks | 6.24± 0.44** | 3.64± 0.07*** | 5.34± 0.06*** | 84.50± 2.23* | *Parmelia perlata* (800 mg/kg body wt./day) at peri, peri, post initiational stages of papillomagenesis |




Group I: CONTOL- 16 weeks duration

Group II: Pre-initiational stage (800mg/kg body wt./day)

Group III: Peri-initiational stage (800mg/kg body wt./day)

Group IV: Post-initiational stage (800mg/kg body wt./day)

Group V: Throughout-initiational stage (800mg/kg body wt./day)

*Graph 4:* The modulatory effect of 800 mg/kg b.wt/day of *Parmelia perlata* extract on the GSH, LPO, SOD and CAT levels in the tissue of Swiss albino mice after initiation of DMBA, followed 2 weeks later by croton oil treatment (three times in a week) for 14 weeks with or without treatment for *Parmelia perlata*

i. *Preparation of Homogenate for Biochemical Studies*

Animals were killed by cervical dislocation and its dorsal skin was taken off, it was then trimmed into pieces and weighed. For reduced glutathione assay it was homogenized in ice-cold Tris KCl buffer (pH 7.4) to yield a 10% (w/v) homogenate. 0.5ml aliquot of this was used for examining reduced glutathione. For assaying lipid peroxidation the tissue was homogenized in ice-cold 1.15% KCl to yield 10% (w/v) homogenate. For lipid peroxidation assay 0.8 ml aliquot was used.

Reduced glutathione (GSH): GSH is total non-protein sulphydryl group which is estimated by the method [32]. Absorbance was read against blank at 412 nm wavelength using UV-VIS Systronics spectro-photometer [33]. Absorbance was taken at 532 nm wavelength using UV-VIS Systronics spectro-photometer.

*d) Statistical Analysis*

i. *Study parameters*

Statistical significance of difference between control and experimental groups were determined by Student's t- test and Analysis of variance (ANNOVA) test.

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*Plate - I*

*Fig. 1:* Normal unclipped male *Swiss albino* mice

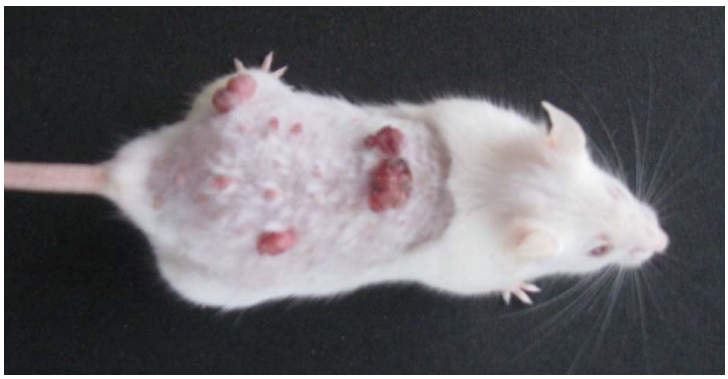

*Fig. 2:* Male *Swiss albino* mice with papillomas developed on the dorsal side after topical application of 7, 12-dimethylbenz(a) anthracene (DMBA) and croton oil

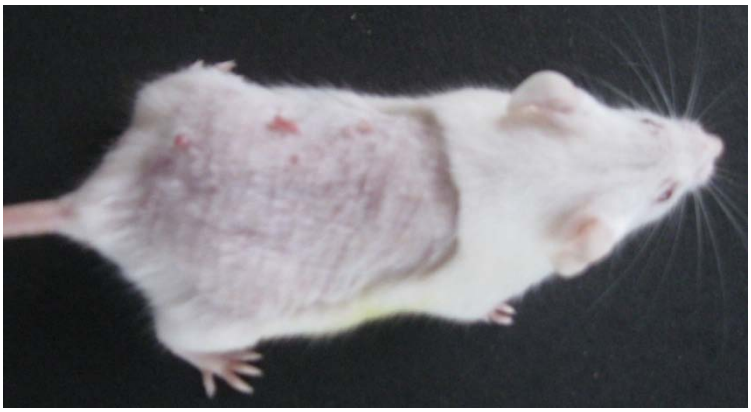

*Fig. 3:* Reduced number of papillomas were displayed by the mice treated orally with *Parmelia perlata* extract at a dose level of (800 mg/kg body wt./day)

# Global Journals Guidelines Handbook 2020

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# Memberships

## Fellows/Associates of Science Frontier Research Council

### FSFRC/ASFRC Memberships

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FSFRC/ASFRC is the most prestigious membership of Global Journals accredited by Open Association of Research Society, U.S.A (OARS). The credentials of Fellow and Associate designations signify that the researcher has gained the knowledge of the fundamental and high-level concepts, and is a subject matter expert, proficient in an expertise course covering the professional code of conduct, and follows recognized standards of practice. The credentials are designated only to the researchers, scientists, and professionals that have been selected by a rigorous process by our Editorial Board and Management Board.

Associates of FSFRC/ASFRC are scientists and researchers from around the world are working on projects/researches that have huge potentials. Members support Global Journals' mission to advance technology for humanity and the profession.

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FELLOW OF SCIENCE FRONTIER RESEARCH COUNCIL is the most prestigious membership of Global Journals. It is an award and membership granted to individuals that the Open Association of Research Society judges to have made a 'substantial contribution to the improvement of computer science, technology, and electronics engineering.

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| Associate | Fellow | Research Group | Basic |
|---|---|---|---|
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2. Drafting the paper and revising it critically regarding important academic content.
3. Final approval of the version of the paper to be published.

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**Acknowledgments**

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The following is the official style and template developed for publication of a research paper. Authors are not required to follow this style during the submission of the paper. It is just for reference purposes.

***Manuscript Style Instruction (Optional)***

- Microsoft Word Document Setting Instructions.
- Font type of all text should be Swis721 Lt BT.
- Page size: 8.27" x 11'", left margin: 0.65, right margin: 0.65, bottom margin: 0.75.
- Paper title should be in one column of font size 24.
- Author name in font size of 11 in one column.
- Abstract: font size 9 with the word "Abstract" in bold italics.
- Main text: font size 10 with two justified columns.
- Two columns with equal column width of 3.38 and spacing of 0.2.
- First character must be three lines drop-capped.
- The paragraph before spacing of 1 pt and after of 0 pt.
- Line spacing of 1 pt.
- Large images must be in one column.
- The names of first main headings (Heading 1) must be in Roman font, capital letters, and font size of 10.
- The names of second main headings (Heading 2) must not include numbers and must be in italics with a font size of 10.

***Structure and Format of Manuscript***

The recommended size of an original research paper is under 15,000 words and review papers under 7,000 words. Research articles should be less than 10,000 words. Research papers are usually longer than review papers. Review papers are reports of significant research (typically less than 7,000 words, including tables, figures, and references)

A research paper must include:

a) A title which should be relevant to the theme of the paper.
b) A summary, known as an abstract (less than 150 words), containing the major results and conclusions.
c) Up to 10 keywords that precisely identify the paper's subject, purpose, and focus.
d) An introduction, giving fundamental background objectives.
e) Resources and techniques with sufficient complete experimental details (wherever possible by reference) to permit repetition, sources of information must be given, and numerical methods must be specified by reference.
f) Results which should be presented concisely by well-designed tables and figures.
g) Suitable statistical data should also be given.
h) All data must have been gathered with attention to numerical detail in the planning stage.

Design has been recognized to be essential to experiments for a considerable time, and the editor has decided that any paper that appears not to have adequate numerical treatments of the data will be returned unrefereed.

i) Discussion should cover implications and consequences and not just recapitulate the results; conclusions should also be summarized.
j) There should be brief acknowledgments.
k) There ought to be references in the conventional format. Global Journals recommends APA format.

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The Editorial Board reserves the right to make literary corrections and suggestions to improve brevity.

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The title page must carry an informative title that reflects the content, a running title (less than 45 characters together with spaces), names of the authors and co-authors, and the place(s) where the work was carried out.

**Author details**

The full postal address of any related author(s) must be specified.

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The abstract is the foundation of the research paper. It should be clear and concise and must contain the objective of the paper and inferences drawn. It is advised to not include big mathematical equations or complicated jargon.

Many researchers searching for information online will use search engines such as Google, Yahoo or others. By optimizing your paper for search engines, you will amplify the chance of someone finding it. In turn, this will make it more likely to be viewed and cited in further works. Global Journals has compiled these guidelines to facilitate you to maximize the web-friendliness of the most public part of your paper.

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A major lynchpin of research work for the writing of research papers is the keyword search, which one will employ to find both library and internet resources. Up to eleven keywords or very brief phrases have to be given to help data retrieval, mining, and indexing.

One must be persistent and creative in using keywords. An effective keyword search requires a strategy: planning of a list of possible keywords and phrases to try.

Choice of the main keywords is the first tool of writing a research paper. Research paper writing is an art. Keyword search should be as strategic as possible.

One should start brainstorming lists of potential keywords before even beginning searching. Think about the most important concepts related to research work. Ask, “What words would a source have to include to be truly valuable in a research paper?” Then consider synonyms for the important words.

It may take the discovery of only one important paper to steer in the right keyword direction because, in most databases, the keywords under which a research paper is abstracted are listed with the paper.

**Numerical Methods**

Numerical methods used should be transparent and, where appropriate, supported by references.

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Authors must list all the abbreviations used in the paper at the end of the paper or in a separate table before using them.

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Authors are advised to submit any mathematical equation using either MathJax, KaTeX, or LaTeX, or in a very high-quality image.

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Tables: Tables should be cautiously designed, uncrowned, and include only essential data. Each must have an Arabic number, e.g., Table 4, a self-explanatory caption, and be on a separate sheet. Authors must submit tables in an editable format and not as images. References to these tables (if any) must be mentioned accurately.

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Although low-quality images are sufficient for review purposes, print publication requires high-quality images to prevent the final product being blurred or fuzzy. Submit (possibly by e-mail) EPS (line art) or TIFF (halftone/ photographs) files only. MS PowerPoint and Word Graphics are unsuitable for printed pictures. Avoid using pixel-oriented software. Scans (TIFF only) should have a resolution of at least 350 dpi (halftone) or 700 to 1100 dpi (line drawings). Please give the data for figures in black and white or submit a Color Work Agreement form. EPS files must be saved with fonts embedded (and with a TIFF preview, if possible).

For scanned images, the scanning resolution at final image size ought to be as follows to ensure good reproduction: line art: >650 dpi; halftones (including gel photographs): >350 dpi; figures containing both halftone and line images: >650 dpi.

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***12. Know what you know:*** Always try to know what you know by making objectives, otherwise you will be confused and unable to achieve your target.

***13. Use good grammar:*** Always use good grammar and words that will have a positive impact on the evaluator; use of good vocabulary does not mean using tough words which the evaluator has to find in a dictionary. Do not fragment sentences. Eliminate one-word sentences. Do not ever use a big word when a smaller one would suffice.

Verbs have to be in agreement with their subjects. In a research paper, do not start sentences with conjunctions or finish them with prepositions. When writing formally, it is advisable to never split an infinitive because someone will (wrongly) complain. Avoid clichés like a disease. Always shun irritating alliteration. Use language which is simple and straightforward. Put together a neat summary.

***14. 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 for your topic. You may also maintain your arguments with records.

***15. Never start at the last minute:*** Always allow enough time for research work. Leaving everything to the last minute will degrade your paper and spoil your work.

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

***17. Never copy others' work:*** Never copy others' work and give it your name because if the evaluator has seen it anywhere, you will be in trouble. Take proper rest and food: No matter how many hours you spend on your research activity, if you are not taking care of your health, then all your efforts will have been in vain. For quality research, take proper rest and food.

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

***19. Refresh your mind after intervals:*** Try to give your mind a rest by listening to soft music or sleeping in intervals. This will also improve your memory. Acquire colleagues: Always try to acquire colleagues. No matter how sharp you are, if you acquire colleagues, they can give you ideas which will be helpful to your research.

***20. Think technically:*** Always think technically. If anything happens, search for its reasons, benefits, and demerits. Think and then print: When you go to print your paper, check that tables are not split, headings are not detached from their descriptions, and page sequence is maintained.

***21. Adding unnecessary information:*** Do not add unnecessary information like "I have used MS Excel to draw graphs." Irrelevant and inappropriate material is superfluous. Foreign terminology and phrases are not apropos. One should never take a broad view. Analogy is like feathers on a snake. Use words properly, regardless of how others use them. Remove quotations. Puns are for kids, not grunt readers. Never oversimplify: When adding material to your research paper, never go for oversimplification; this will definitely irritate the evaluator. Be specific. Never use rhythmic redundancies. Contractions shouldn't be used in a research paper. Comparisons are as terrible as clichés. Give up ampersands, abbreviations, and so on. Remove commas that are not necessary. Parenthetical words should be between brackets or commas. Understatement is always the best way to put forward earth-shaking thoughts. Give a detailed literary review.

***22. Report concluded results:*** Use concluded results. From raw data, filter the results, and then conclude your studies based on measurements and observations taken. An appropriate number of decimal places should be used. Parenthetical remarks are prohibited here. Proofread carefully at the final stage. At the end, give an outline to your arguments. Spot perspectives of further study of the subject. Justify your conclusion at the bottom sufficiently, which will probably include examples.

***23. Upon 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 for 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 of 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 criteria peer reviewers will use for grading the final paper.

**Final points:**

One purpose of organizing a research paper is to let people interpret your efforts selectively. The journal requires the following sections, submitted in the order listed, with each section starting on a new page:

*The introduction:* This will be compiled from reference matter and reflect the design processes or outline of basis that directed you to make a study. As you carry out the process of study, the method and process section will be constructed like that. The results segment will show related statistics in nearly sequential order and direct reviewers to similar intellectual paths throughout the data that you gathered to carry out your study.

**The discussion section:**

This will provide understanding of the data and projections as to the implications of the results. The use of good quality references throughout the paper will give the effort trustworthiness by representing an alertness to 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 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 avoid:*

- Insertion of a title at the foot of a page with subsequent text on the next page.
- Separating a table, chart, or figure—confine each to a single page.
- Submitting a manuscript with pages out of sequence.
- In every section of your document, use standard writing style, including articles ("a" and "the").
- Keep paying attention to the topic of the paper.
- Use paragraphs to split each significant point (excluding the abstract).
- Align the primary line of each section.
- Present your points in sound order.
- Use present tense to report well-accepted matters.
- Use past tense to describe specific results.
- Do not use familiar wording; don't address the reviewer directly. Don't use slang or superlatives.
- Avoid use of extra pictures—include only those figures essential to presenting results.

**Title page:**

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

**Abstract:** This summary should be two hundred words or less. It should clearly and briefly explain the key findings reported in the manuscript and must have precise statistics. It should not have acronyms or abbreviations. It should be logical in itself. Do not cite 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 approaches 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. Use comprehensive sentences, and do not sacrifice readability for brevity; you can maintain it succinctly by phrasing sentences so that they provide more than a 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 limit the initial two items to no more than one line each.

*Reason for writing the article—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 for this; results of any numerical analysis should be reported. Significant conclusions or questions that emerge from the research.

**Approach:**

- Single section and succinct.
- An outline of the job done is always written in past tense.
- Concentrate on shortening results—limit background information to a verdict or two.
- Exact spelling, clarity 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 of comprehending and calculating the purpose of your study without having to refer to other works. The basis for the study should be offered. Give the most important references, but avoid making a comprehensive appraisal of the topic. Describe the problem visibly. If the problem is not acknowledged in a logical, reasonable way, the reviewer will give no attention to your results. Speak in common terms about techniques used to explain the problem, if needed, but do not present any particulars about the protocols here.

*The following approach can create a valuable beginning:*

- Explain the value (significance) of the study.
- Defend the model—why did you employ this particular system or method? What is its compensation? Remark upon its appropriateness from an abstract point of view as well as pointing out sensible reasons for using it.
- Present a justification. State your particular theory(-ies) or aim(s), and describe the logic that led you to choose them.
- Briefly explain the study's tentative purpose and how it meets the declared objectives.

**Approach:**

Use past tense except for when referring to recognized facts. After all, the manuscript will be submitted after the entire job is done. Sort out your thoughts; manufacture one key point for every section. If you make the four points listed above, you will need at least four paragraphs. Present surrounding information only when it is necessary to support a situation. The reviewer does not desire to read everything you know about a topic. Shape the theory 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 soundly written procedures segment allows a capable scientist to replicate 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 to give the least amount of information that would permit another capable scientist to replicate 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 section, mention the specific item describing the way, but draw the basic principle while stating the situation. The purpose is to show 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:**

*Materials may be reported in part of a section or else they may be recognized along with your measures.*

**Methods:**

- Report the method and not the 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—detail how procedures were completed, not how they were performed on a particular day.
- If well-known procedures were used, account for the procedure by name, possibly with a reference, and that's all.

**Approach:**

It is embarrassing to use vigorous voice when documenting methods without using first person, which would focus the reviewer's interest on the researcher rather than the job. As a result, when writing up the methods, most authors use third person passive voice.

Use standard style in this and 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 as 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. Use statistics and tables, if suitable, to present consequences most efficiently.

You must clearly differentiate material which would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matters should not be submitted at all except if requested by the instructor.

**Content:**

- Sum up your conclusions in text and demonstrate them, if suitable, with figures and tables.
- In the manuscript, explain each of your consequences, and point the reader to remarks that are most appropriate.
- Present a background, such as by describing the question that was addressed by creation of an exacting study.
- Explain results of control experiments and give 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 manuscript.

**What to stay away from:**

- Do not discuss or infer your outcome, report surrounding information, or try to explain anything.
- Do not include raw data or intermediate calculations in a research manuscript.
- Do not present similar data more than once.
- A manuscript should complement any figures or tables, not duplicate information.
- Never confuse figures with tables—there is a difference.

**Approach:**

As always, use past tense when you submit 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 section.

**Figures and tables:**

If you put figures and tables at the end of some details, make certain that they are visibly distinguished from any attached appendix materials, such as raw facts. Whatever the position, each table must be titled, numbered one after the other, and include a heading. All figures and tables must be divided from the text.

**Discussion:**

The discussion is expected to be the trickiest segment to write. A lot of papers submitted to the journal are discarded based on problems with the discussion. There is no rule for how long an 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 implications of the study. The purpose here is to offer an understanding of your results and support all of your conclusions, using facts from your research and generally accepted information, if suitable. The implication of results should be fully 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 the prospect, and let it drop at that. Make a decision as to whether each premise is supported or 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 an experiment might be personalized to accomplish a new idea.
- Give details of all of your remarks as much as possible, focusing on mechanisms.
- Make a decision as to whether the tentative design sufficiently addressed the theory and whether or not it was correctly restricted. Try to present substitute explanations if they are sensible alternatives.
- One piece of 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 other available information. Present work done by specific persons (including you) in past tense.

Describe generally acknowledged facts and main beliefs in present tense.

## The Administration Rules

Administration Rules to Be Strictly Followed before Submitting Your Research Paper to Global Journals Inc.

*Please read the following rules and regulations carefully before submitting your research paper to Global Journals Inc. to avoid rejection*.

*Segment draft and final research paper:* You have to strictly follow the template of a research paper, failing which your paper may get rejected. You are expected to write each part of the paper wholly on your own. The peer reviewers need to identify your own perspective of the concepts in your own terms. Please do not extract straight from any other source, and do not rephrase someone else's analysis. Do not allow anyone else to proofread your manuscript.

*Written material:* You may discuss this with your guides and key sources. Do not copy anyone else's paper, even if this is only imitation, otherwise it will be rejected on the grounds of plagiarism, which is illegal. Various methods to avoid plagiarism are strictly applied by us to every paper, and, if found guilty, you may be blacklisted, which could affect your career adversely. To guard yourself and others from possible illegal use, please do not permit anyone to use or even read your paper and file.

## Criterion for Grading a Research Paper (Compilation) by Global Journals

**Please note that following table is only a Grading of "Paper Compilation" and not on "Performed/Stated Research" whose grading solely depends on Individual Assigned Peer Reviewer and Editorial Board Member. These can be available only on request and after decision of Paper. This report will be the property of Global Journals.**

| 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<br><br>Above 200 words | No specific data with ambiguous information<br><br>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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