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Evaluation of Adulteration

Stresses Relaxation Mechanism

Highlights

Determination of Bromethalin

Theoretical Analysis of Reactivity

Discovering Thoughts, Inventing Future

VOLUME 17 ISSUE 1 VERSION 1.0

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Stresses Relaxation Mechanism in the Si-Sio$_2$ System and its Influence on the Interface Properties

By Daniel Kropman, Tõnu Laas, Viktor Seeman & Artur Medvids
Tallinn University

Abstract- The results of the investigation of stresses relaxation by strain by means of EPR spectra, IR absorption spectra, SEM and samples deflection are presented. It has been shown that stresses relaxation mechanism depended on the oxidation condition: temperature, cooling rate, oxide thickness. In the Si-SiO_2-Si_3N_4 system the stresses relaxation by the strain occur due to the opposite sign of the thermal expansion coefficient of Si-SiO_2 and Si_3N_4 on Si. Laser irradiation allows to modify the system stresses.

Keywords: *Si-SiO_2 interface, stress relaxation, EPR, SEM.*

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Stresses Relaxation Mechanism in the Si-Sio_2 System and its Influence on the Interface Properties

Daniel Kropman [α], Tõnu Laas [σ], Viktor Seeman [ρ] & Artur Medvids [ω]

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Keywords: *Si-SiO_2 interface, stress relaxation, EPR, SEM.*

I. Introduction

It is known that internal mechanical stresses due to the differences in the thermal expansion coefficient between films and substrates and lattices mismatch appear in the Si-SiO_2 system during the process of its formation and that point defects generation and redistribution reduce partially the surface strain. However, no investigation of this process on the atomic scale has been carried out so far. The purpose of the present work is to investigate the strain relaxation mechanism in the Si-SiO_2 system by means of EPR, IR absorption spectroscopy, scanning electron microscopy (SEM) and samples bending measurements.

II. Experimental

Si n-type with 15 Ω·cm resistivity and (111) orientation was used. The oxides were thermally grown in dry oxygen at 1100-1200 °C. The SiO_2 film thickness varied from 0.2 μm to about 0,5 μm. The density of point defects was varied by varying the cooling rate of the samples (3 of 25 °C/s). The EPR spectra were taken at 115 K by an X-band ESR 231 spectrometer. To evaluate the influence of the defects structure on the stresses in SiO_2, the measurements of SiO_2 IR absorption spectra were carried out. The strain in the Si-SiO_2 system were investigated by means of SEM and samples bending measurements. Laser irradiation (λ=520nm, 10mW/cm^2) were performed after oxidation.

III. Results and Discussion

It has been found that samples bending increases or decreases simultaneously with EPR signal intensity depending on the oxidation temperature, oxidation time and cooling rate.(Fig.1) It may be due to the relaxation of stresses by the strain accompanied by the point defects gettering and by creation of point defects by the stresses. It has been found that in case of a lower oxidation temperature (1100^{0}C) the deflection of the samples decreases with an increase of the EPR signal intensity (E`centres in SiO_2 and vacancy complexes in Si) while at a higher oxidation temperature (1200^{0}C) the deflection of the samples and EPR signal intensity increase simultaneously[1,2]. The revealed differences in the strain dependence on the point defects density (type) at different oxidation temperature allow to suggest that relaxation mechanism of the internal mechanical stresses (IMS) is different. During oxidation at 1100^{0}C oxygen diffuses through the oxide to the interface where oxidation happens which is associated with a volume expansion. Part of the volume is released by injection of Si self-interstitials into the Si. At 1200^{0}C diffusion of Si from the interface into the oxide occurs and the oxidation reaction happens in the oxide. This process is associated with vacancy injection into the Si. The decrease of the deflection with an increase of the vacancies type point defects EPR signal intensity indicates that self-interstitial Si atoms injection are responsible for the stresses in the samples oxidized at 1100^{0}C. This oxidation kinetics model is in agreement with point defects generation kinetics in the Si-SiO_2 system proposed in [3] and confirmed experimentally [4]. It has been suggested that the incorporation of the ionic charge into the oxide cause repulsive forces expanding the silicon wafer [5]. This allows one to explain this simultaneous increase of the E` centers EPR signal intensity and deflection in samples oxidized at 1200$^0$C. E`centers cause repulsive forces expanding the Si wafer and giving rise for the deflection in Si-SiO_2 structure.

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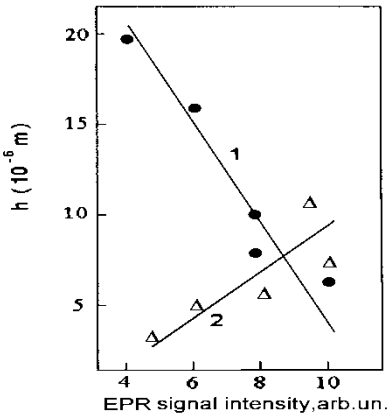

Fig. 1: Relation between the deflection of samples and EPR signal of Pa centers for the samples oxidized at 1100 (1) and 1200°C (2)

At an appropriate choose of the oxidation temperature tensile stresses in Si and compressive stresses in SiO_2 can be equal and canceled out.To find thise temperature oxidation at 1120,1130 and 1140^0 C were performed. With an increase of the oxidation temperature the thickness of the oxide layer decreases.This can be explained by the increase of tensile stresses in Si and decrease of compressive stresses in SiO_2. Absent of defects on crossection of samples prepared at oxidation temperature 1130^{0}C (Fig.4) confirm this assumption.

To evaluate the strain dependence on the SiO_2 film thickness the EPR signal and IR absorbtion at 1100 cm^{-1} line-width were measured (2). EPR signal dependence on the oxidation time reveal one or two maximum depending on the cooling rate. In fast-cooled samples there exist a interdependence between EPR signal and IR absorption line-width at 1100cm^{-1}($\Delta\nu$). In slowly cooled samples the increase of the EPR signal is accompanied by the decrease of $\Delta\nu$ that indicated stress dependence on SiO_2 film thickness.In samples with SiO_2 thicness >0.4 μm point defects density decreasing in Si is accompanied by $\Delta\nu$ increase.This may be explained by O inclussion formation in Si.In samples with SiO_2 film thickness ~ 0,2 and ~ 0,4 μm absent of cooling rate influence on point defects density and $\Delta\nu$ allow to suggest IMS absent.

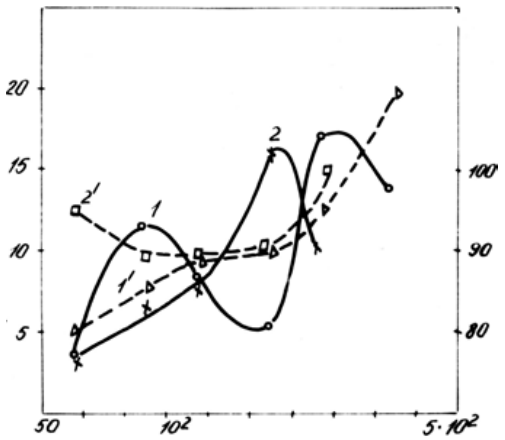

Fig. 2: Dependence of the EPR signal (1, 2) and the line-width of SiO_2 IR absorption at 1100 cm-1 (1', 2') on the oxidation time, cooling rate 25 (1, 1') and 3°Cs (2, 2')

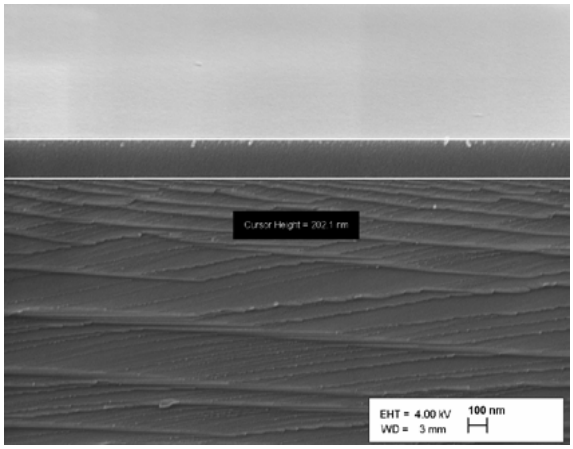

Fig. 3: Si-SiO2 cross-section micrograph, oxidation temperature 1120oC.

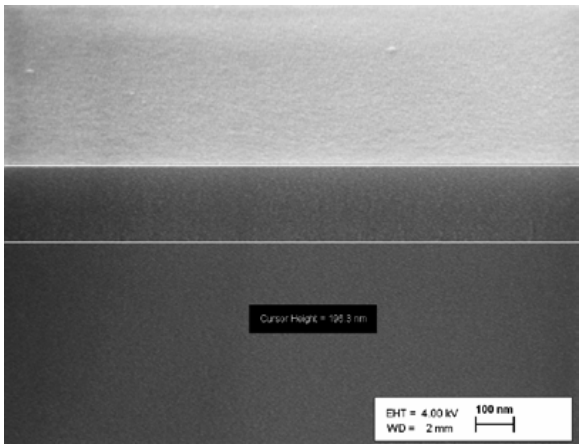

Fig.4: Si-SiO_2 cross-section micrograph, oxidation temperature 1130°C

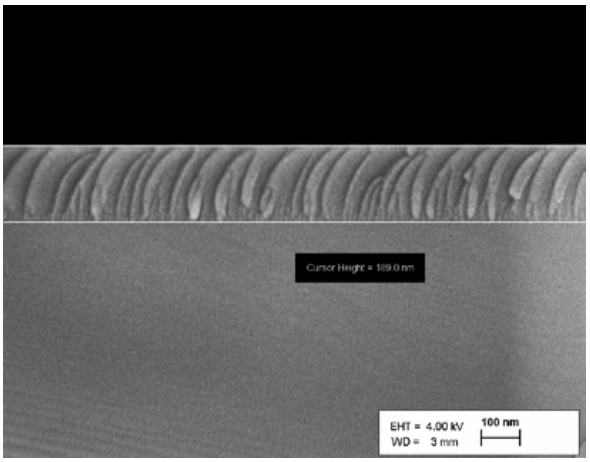

Fig. 5: Si-SiO_2 cross-section micrograph, oxidation temperature 1140°C

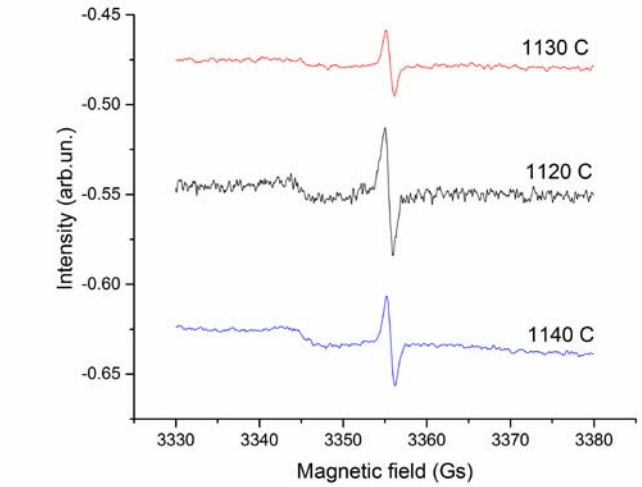

Fig. 6: EPR spectra of Si(n)-SiO_2 sample obtained at different oxidation temperatures

In Fig.6 EPR spectra of samples obtained at different oxidation temperature is shown.

It can be seen, that in n-type silicon samples obtained at 1130^0 C both centers (vacancies complexes and unsaturated bonds) EPR signal intensity is lower than in samples obtained at 1120 and 1140^{0}C.
This confirm lower IMS at these oxidation temperature.

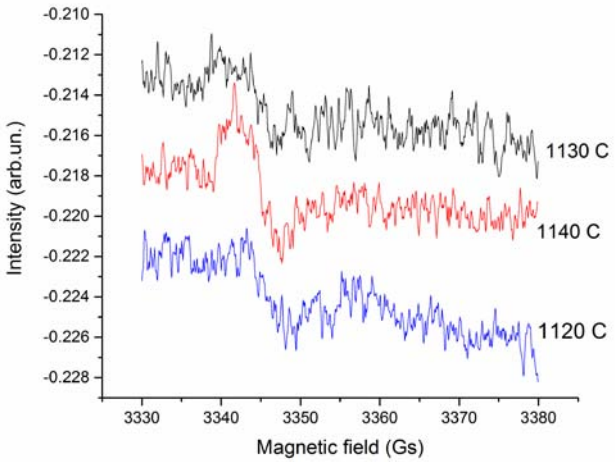

Fig. 7: EPR spectra of Si(p)-SiO_2 sample obtained at different oxidation temperatures

It can be seen that the oxidation temperature influence on generation of defects in p-type samples is lower than in case of n-type Si samples. The influence of oxidation temperature on vacancies is absent,and the influence on unsaturated bonds is the same as for n-type Si samples. Differences between n-type and p-type Si can be due to the different stresses in n- and p-type Si samples.Different deflection in Si(p)-SiO_2 and Si(n)-SiO_2 confirm thise assumption.

IV. Conclusion

The obtained results confirm that there exists an interdependence between the stresses created in the Si-SiO_2 structure and point defects in Si and SiO_2. It has been shown that at oxidation temperature 1130^{0}C performed Si-SiO_2 structures IMS canceled out. It has been established that the dependence of the EPR signal intensity from vacancy type defects on the oxidation time is non-monotonous and is accompanied by a non-monotonous change of the IMS. In samples with SiO_2 film thickness 0.2-0.4 μm IMS at the Si-SiO_2 interface dissapear. It was observed that dependence of EPR signal of Si(n)-SiO_2 and Si(p)-SiO_2 samples obtained at different oxidation temperatures was different. It can be concluded that this is related to different mechanical stresses in the n-type and p-type Si-SiO_2 samples.

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Theoretical Analysis of Reactivity and Regioselectivity in [1+2] Cycloaddtion Reaction of Some Monoterpenes with Dichlorocarbene

By A. Zeroual, M. Zoubir, M. El Idrissi, R. El ajlaoui, A. El Haib, S. Abouricha, N. Mazoir & A. El Hajbi
Chouaïb Doukkali University

Abstract- A theoretical study of the molecular mechanism and regioselectivity of the [1+2] cycloaddition reaction between alkenes: limonene, terpinolene, γ-terpinene and dichlorocarbene has been carried out at the B3LYP/6-31G (d,p) level of theory. The calculation of activation and reaction free energies indicates that these reactions are regio-specific in good agreement with experimental result.

Keywords: [1+2] cycloaddition, limonene, terpinolene, γ-terpinene, DFT/6-31(d, p), TST.

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Theoretical Analysis of Reactivity and Regioselectivity in [1+2] Cycloaddtion Reaction of Some Monoterpenes with Dichlorocarbene

A. Zeroual [α], M. Zoubir [σ], M. El Idrissi [ρ], R. El ajlaoui [ω], A. El Haib [¥], S. Abouricha [§], N. Mazoir [χ] & A. El Hajbi [ν]

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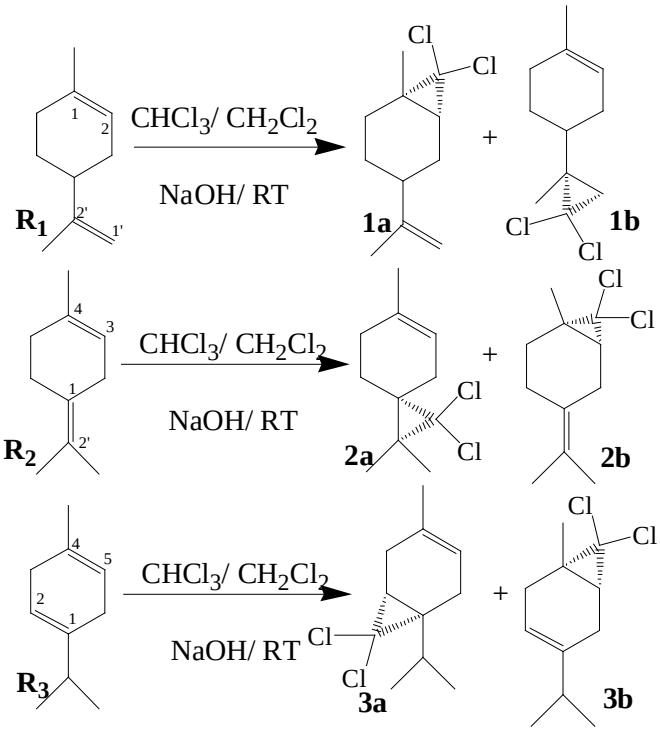
Keywords: [1+2] cycloaddition, limonene, terpinolene, γ-terpinene, DFT/6-31(d, p), TST.

I. Introduction

The monoterpenes are essential ingredients in fine chemical industry and flavor and perfume industry. It is used to flavour many kinds of baked goods, confections, pudding, meats, sausages, sauces, vegetables and beverages [1]. The pharmacological activities of nutmeg mainly exist in its essential oil fraction [2]. Nutmeg oil possesses a wide array of pharmacological actions including analgesic [3], antifungal [4-7], antimicrobial [8-12], anti-inflammatory [13], antibacterial [14-16], antioxidant [17-18], antidepressant [19], as well as hepatoprotective activity [20]. The most important constituents of monoterpenes are α- and β- pinene. We were interested in a classical reactivity of carbenes. The dichlorocarbene reacts with alkenes such as limonene R_1 (4-Isopropenyl-1-methyl-cyclohexene), terpinolene R_2 (4-Isopropylidene-1-methyl-cyclohexene) and γ-terpinene R_3 (1-Isopropyl-4-methyl-cyclohexa-1,4-diene) in dichloromethane, to form the cyclopropane derivative (Scheme 1). The structures of these products have been determined by spectroscopy (^{1}H, ^{13}C and mass spectroscopy). [21]



Scheme 1: [1+2] cycloaddition reaction of limonene 1, terpinolene 2 and γ-terpinene 3 with dichlorocarbene.

Herein, a DFT study of the [1+2] cycloaddition reaction of limonene 1, terpinolene 2 and γ-terpinene 3 with dichlorocarbene yielding: 4-(2-propene)-1-Methyl-7,7-dichloro-bicyclo[4.1.0]heptane, 1,1-Dichloro-2,2,6-trimethyl-spiro[2.5]oct-5-ene and 7,7-Dichloro-4-isopropyl-1-methyl-bicyclo[4.1.0]hept-3-ene,experimentally studied by Hossni Ziyat et al. [21] are presented (see Scheme 1). Our aim is to perform a theoretical study of the reaction mechanism of these cycloaddition reactions yielding the final products: 1a, 2a and 3a, as well as to explain the regioselectivity experimentally observed.

II. Computational Details

All calculations reported in this work were performed in the GAUSSIAN 09, B3LYP/6-31G(d,p) as well as theoretical levels were performed. Optimizations of the stable structures were performed with the Berny

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algorithm, whereas the transition states were calculated using the QST2 procedure followed by the TS method. Stationary points were characterized by frequency calculations. All transition states showed only one negative eigen value in their Hessian matrices. For all reactions, IRC [22] calculations were performed to connect previously computed transition structures with suitable minima. Solvent effects of dichloromethane were taken into account through single point energy calculations using the polarisable continuum model (PCM). [23]

The global electrophilicity index [24] ω, was given by the following expression, $\omega = (\mu^2/2\eta)$, in terms of the electronic chemical potential μ and the chemical hardness η. Both quantities may be approached in terms of the one-electron energies of the frontier molecular orbital HOMO and LUMO, eH and eL, as μ = (eH - eL)/2 and η = (eL - eH), respectively. [25] The empirical nucleophilicity index N, [26] based on the HOMO energies obtained within the Kohn–Sham scheme, [27] and defined as $N = E_{HOMO}(Nu) - E_{HOMO}(TCE)$. The nucleophilicity was referred to tetracyanoethylene (TCE). Electrophylic P_k^+ and nucleophilic P_k^- Parr functions, [28-34] were obtained through the analysis of the Mulliken atomic spin density (ASD) of the radical anion and radial cation of the reagents. The local electrophilicity and nucleophilicity indices, were evaluated using the following expressions: $\omega_k = \omega . P_k^+$, $N_k = N . P_k^-$

III. Results and Discussion

The present theoretical study is divided into three parts: (i) first, an analysis of DFT reactivity indices at the ground state of the reagents involved in the [1+2] cycloaddition reaction between dichlorocarbene and limonene **1**, terpinolene **2** and γ-terpinene **3** is performed in order to explain the reactivity in these reactions; (ii) in the second part, potential energy surfaces (PESs) are analyzed (iii) in the third part, we proposed new method to calculate the percentages of the products.

a) DFT analysis based on the global and local reactivity indexes

These [1+2] CA reactions were first analyzed using the reactivity indices. The global indices, named electronic chemical potential μ, chemical hardness η, global electrophilicity w and global nucleophilicity N, for the reagents involved in these [1+2] CA reactions are gathered in Table 1.

Table 1: DFT/B3LYP/6-31G (d,p) Electronic chemical potential μ, chemical hardness η, electrophilicity ω, and nucleophilicity N values, in eV

	μ	η	N	ω
limonene **1**	-3.17	5.85	3.42	0.85
terpinolene **2**	-2.46	6.60	3.76	0.45
γ-terpinene **3**	-2.55	6.66	3.63	0.49
Dichlorocarbene **4**	-5.45	3.80	2.17	3.90

The electronic chemical potential of dichlorocarbene, μ= -5.45 eV, is lower than that of limonene **1**, μ= -3.17 eV, terpinolene **2** μ= -2.46 eV and γ-terpinene **3**, μ= -2.55eV, indicating that the global electron density transfer (GEDT) along the corresponding reactions will flux from these the alkenes toward the dichlorocarbene. It also is clear from the table 1 that the dichlorocarbene presents a high electrophilicity w index, w= 3.90 eV, being classified as a strong electrophile and a very low nucleophilicity N index, N= 2.17 eV. On the other hand, limonene **1**, terpinolene **2** and γ-terpinene **3** present very low electrophilicity, w= 0.85 eV, w= 0.45 eV and w= 0.49 eV respectively, and nucleophilicity indices, N= 3.42 eV, N= 3.76 eV and N = 3.63 eV. In spite of the high nucleophilic character of these alkenes (limonene **1**, terpinolene **2** and γ-terpinene), the high electrophilic character of dichlorocarbene allows the participation of these alkynes (limonene **1**, terpinolene **2** and γ-terpinene) in cycloaddition reactions [1+2] as nucleophiles.

The most favourable reactive channel is that involving the initial two-centre interaction between the most electrophilic P_k^+ and nucleophilic P_k^- Parr functions centre of both reagents.

Recently, electrophilic P_k^+ and nucleophilic P_k^- Parr functions have been proposed to analyse the local reactivity in polar processes involving reactions between a nucleophile– electrophile pair.

The analysis of the nucleophilic P_k^- Parr functions of limonene **1**, terpinolene **2** and γ-terpinene **3** (figure 2) shows that the C1 and C2 carbon of limonene **1**, the C1 and C2' carbon of the terpinolene **2** and C1 and C2 carbon of γ-terpinene **3** present the maximum values of P_k^- : 0.22, 0.29, 0.25, 0.27, 0.26 and 0.29 respectively, indicating that these sites are the most nucleophilic centers of these species (see Scheme 1 for atom numbering). Consequently, the regioselectivity observed is predicted correctly by the Parr function.

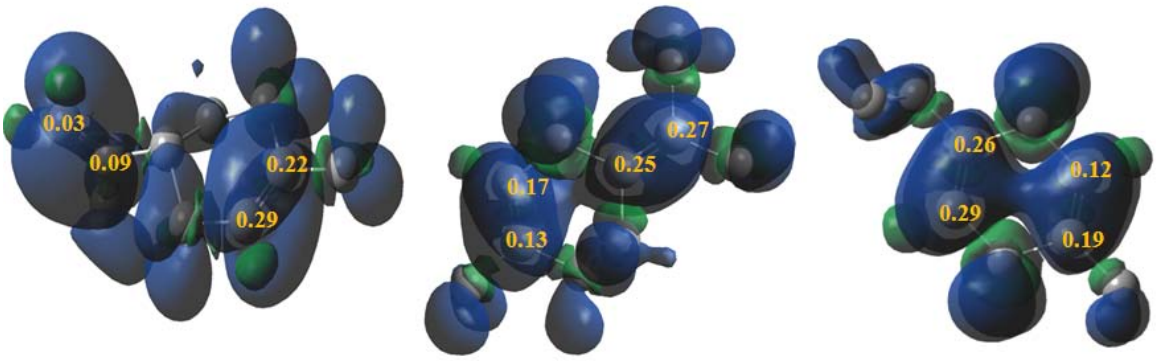


Figure 1: Nucleophilic P_k^- Parr functions of limonene **1**, terpinolene **2** and γ-terpinene **3**

b) Kinetic study

In order to show that the dichlorocarbene preferentially attacks the one double, we calculated the thermodynamic parameters of the reactants, the products and transition states energies, table 2 contains the total and relative enthalpies, entropies, and free energies for the CA [1+2] reaction of the monoterpenes (limonene 1, terpinolene 2 and γ-terpinene 3) and dichlorocarbene.

Table 2: B3LYP/6-31G(d,p) enthalpies H (in a.u.) and relative enthalpies (ΔH, in kcal/mol), entropies S (in cal mol^{-1} K^{-1}) and relative entropies (ΔS, in cal mol^{-1} K^{-1}), free energies G (in a.u.) and relative free energy (ΔG, in kcal/mol) in dichloromethane

System	H	ΔH	G	ΔG	S	ΔS
limonene 1+ CCl_2	-1448.831198	---------	-1448.908944	----------	163.632	----------
TS1a	-1348.849017	-11,181	-1348.908121	**5.165**	124.394	-39,238
TS1b	-1348.833066	-1,172	-1348.892982	**10.016**	126.105	-37,527
1a	-1348.925478	-59,161	-1348.980834	**-45.111**	116.508	-47,124
1b	-1348.905222	-46,450	-1348.957245	**-30.309**	109.492	-54,14
terpinolene 2+ CCl_2	-1448.834525	---------	-1448.913443	----------	166.097	----------
TS2a	-1348.848528	-8,787	-1348.905490	**4.990**	119.885	-46,212
TS2b	-1348.833066	0,915	-1348.892982	**12.839**	126.105	-39,992
2a	-1348.918920	-52,95	-1348.974718	**-38.450**	117.437	-48,66
2b	-1348.914813	-50,381	-1348.967514	**-33.930**	110.919	-55,178
γ-terpinene 3+ CCl_2	-1448.837111	---------	-1448.913249	----------	160.247	----------
TS3a	-1348.843054	-3,729	-1348.900732	**7.854**	121.393	-38,854
TS3b	-1348.834701	1,512	-1348.891202	**13.834**	118.915	-41,332
3a	-1348.913711	-48,0675	-1348.964080	**-31.896**	106.011	-54,236
3b	-1348.906103	-43,293	-1348.959633	**-29.106**	112.663	-47,584

Relative to limonene 1+CCl_2, terpinolene 2+$CCl_2$and γ-terpinene 3+CCl_2

As can be observed, while activation free energies are 5.165 (TS1a), 10.016 (TS1b), 4.990 (TS2a), 12.839 (TS2b), 7.854 (TS3a), and 13.834 (TS3b) kcal mol^{-1}, reaction free energies imply that formation of the corresponding formal [1+2] cycloaddition is highly exothermic; -45.111 (1a), -30.309 (1b), -38.450 (2a), -33.930 (2b), -31.896 (3a) and -29.106 (3b) kcal mol^{-1}. These values clearly indicate that the products 1a, 2a and 3a are preferred.

Using the data given in Table 2, we can sketch the energy profile of these reactions (Fig. 2).

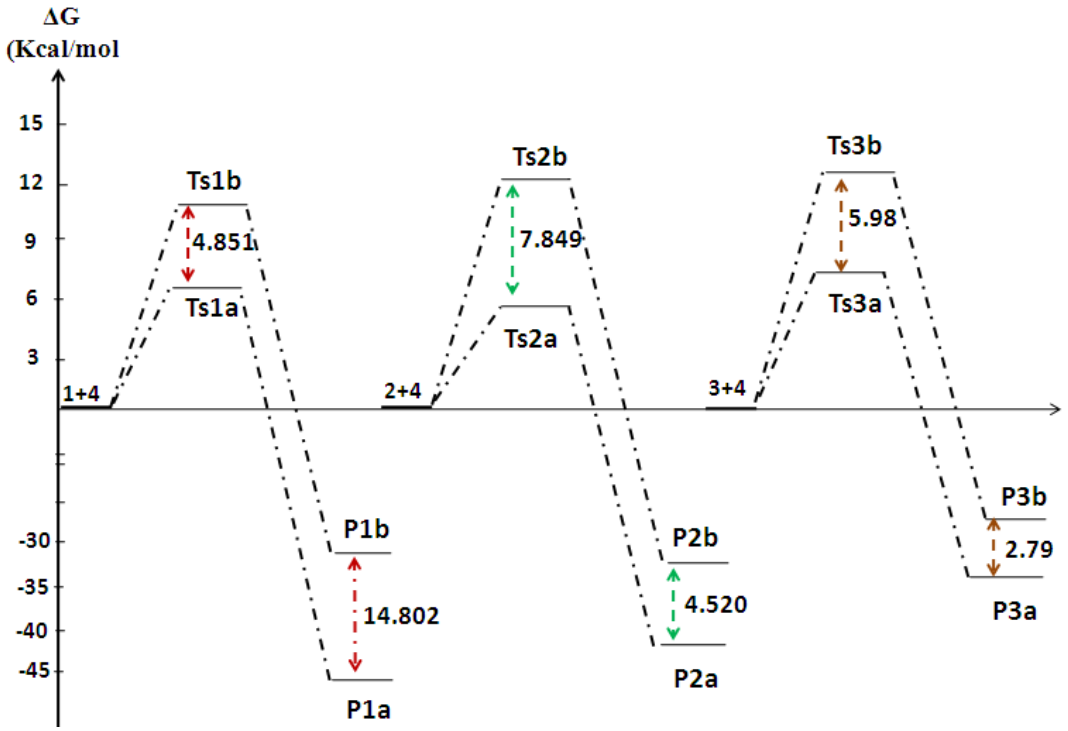
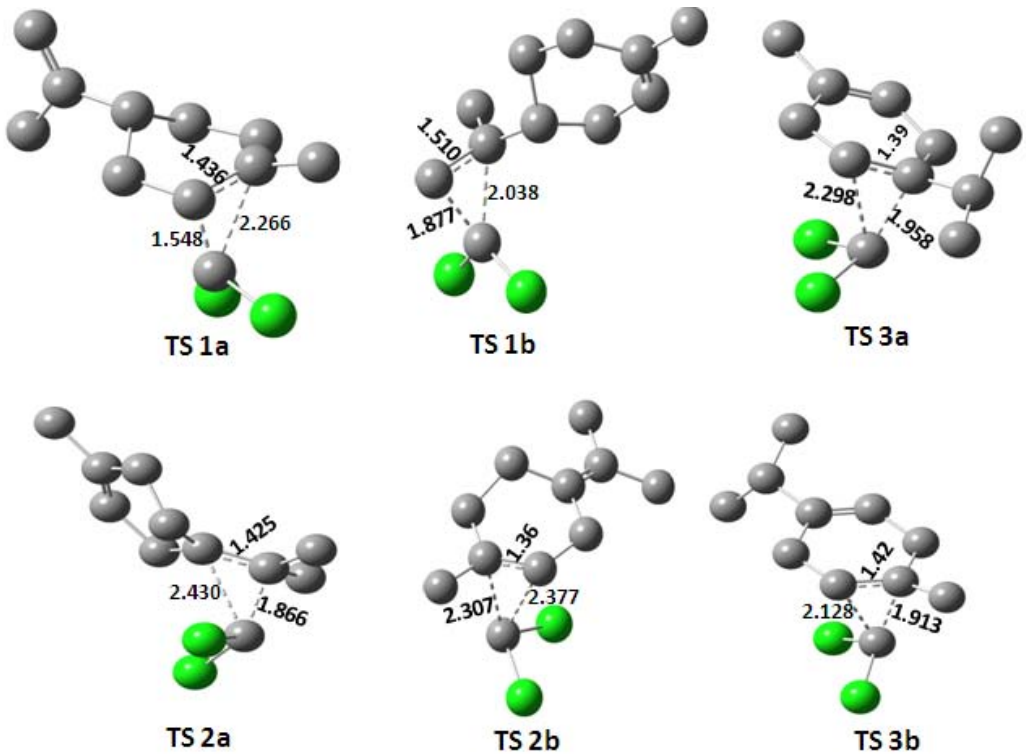


Figure 2: Gibbs free energy profile of [1+2] cycloaddition reaction between dichlorocarbene and alkenes.

We can observed from figure 2 that the deference between activation free energies are 4.851 (Ts1b-Ts1a), 7.849 (Ts2b-Ts2a) and 5.98 (Ts3b-Ts3a), showing that the formation of P1a, P2a and P3a isomers are kinetically preferred. The deference between reaction free energies are 14.802 (1b-1a), 4.520 (2b-2a) and 2.79 (3b-3a), showing that the formation of P1a, P2a and P3a regioisomers are thermodynamically preferred in clears agreement with experimental results.

The optimized geometries of the TSs involved in the studied cycloaddition reaction and the distances of the forming bonds are presented in Figure 3.



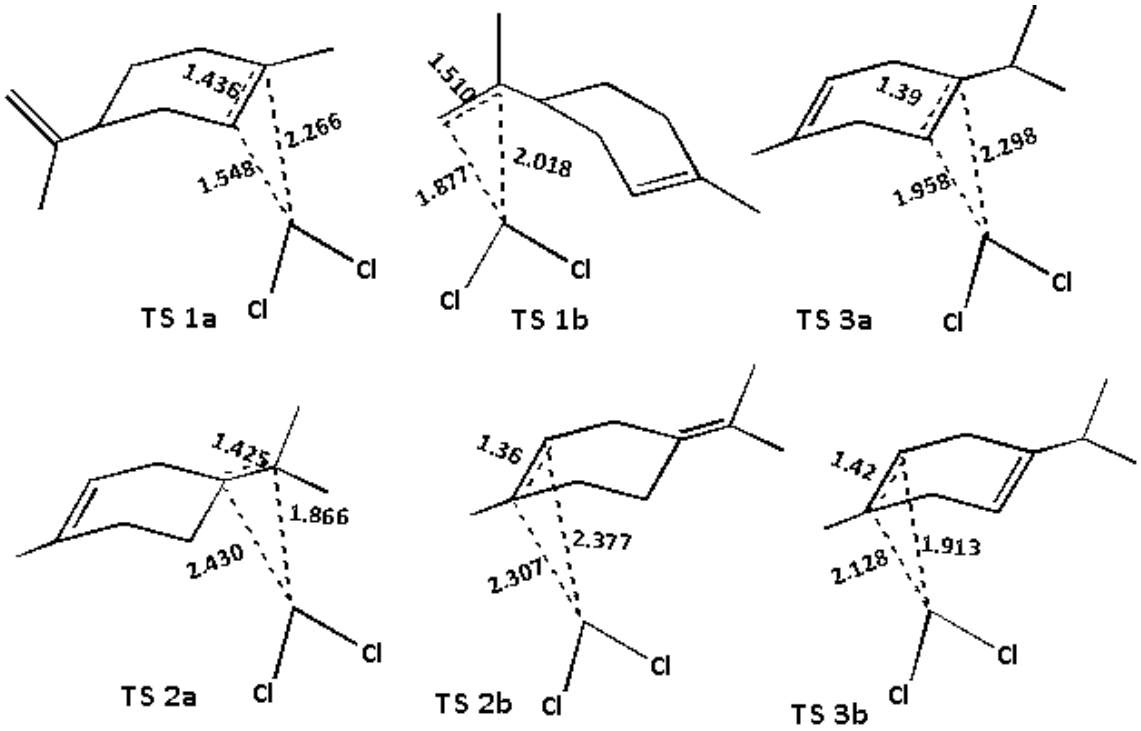


Figure 3: Optimized TS involved in the CA [1+2] reaction of dichlorocarbene–alkene (limonene 1, terpinolene 2 and γ-terpinene 3) the lengths of the newly forming bonds are given in (Å)

c) Calculation of the percentage of the products

According to transition state theory (TST), the second order rate constant (k_{TST}) at a given temperature (T) can be determined using the following equation [35]:

$$K_{TST} = \frac{k_B T}{hC_0} e^{\frac{-\Delta G^{\#}}{RT}} \quad (1)$$

Where k_B, h, C_0, and R denote Boltzmann's constant, Planck's constant, standard concentration (1 mol L^{-1}), and the universal gas constant R = 1,987 cal·K^{-1}·mol^{-1}, respectively.

To calculate the theoretical percentage of the products we use the following equation:

$$\frac{K_{TST}(P1)}{K_{TST}(P2)} = \frac{\frac{k_B T}{hC_0} e^{\frac{-\Delta G^{\#}(P1)}{RT}}}{\frac{k_B T}{hC_0} e^{\frac{-\Delta G^{\#}(P2)}{RT}}}$$

$$= e^{\frac{\Delta G^{\#}(P2)-\Delta G^{\#}(P1)}{RT}} = \frac{\%\, P1}{\%\, P2} = \frac{50+n}{50-n} \qquad with: 0 \le n < 50$$

$$n = \frac{50\left(e^{\frac{\Delta G^{\#}(P2)-\Delta G^{\#}(P1)}{RT}} - 1\right)}{e^{\frac{\Delta G^{\#}(P2)-\Delta G^{\#}(P1)}{RT}} + 1} \quad (2)$$

$$\Delta G^{\#}(P2) - \Delta G^{\#}(P1) = RT Ln\left(\frac{50+n}{50-n}\right) \quad (3)$$

The difference of relative free energy and percentage of the products are reported in table 3.

Table 3: $\Delta G^{\#}(P2) - \Delta G^{\#}(P1)$ Difference of relative free energy (in Kcal/mol) and percentage of the products

n	$\Delta G^{\#}(P2) - \Delta G^{\#}(P1)$	% P1	% P2
0	0	50	50
1	0,0236882	51	49
2	0,04739537	52	48
3	0,07114057	53	47

4	0,09494305	54	46
5	0,11882234	55	45
6	0,14279832	56	44
7	0,1668914	57	43
8	0,19112252	58	42
9	0,21551336	59	41
10	0,24008643	60	40
15	0,36654921	65	35
20	0,50170709	70	30
25	0,6505169	75	25
30	0,82086093	80	20
35	1,02710238	85	15
40	1,3010338	90	10
41	1,3699634	91	9
42	1,44617718	92	8
43	1,53164601	93	7
44	1,6292556	94	6
45	1,74347887	95	5
46	1,8818083	96	4
47	2,05828841	97	3
48	2,30444799	98	2
49	2,72088994	99	1

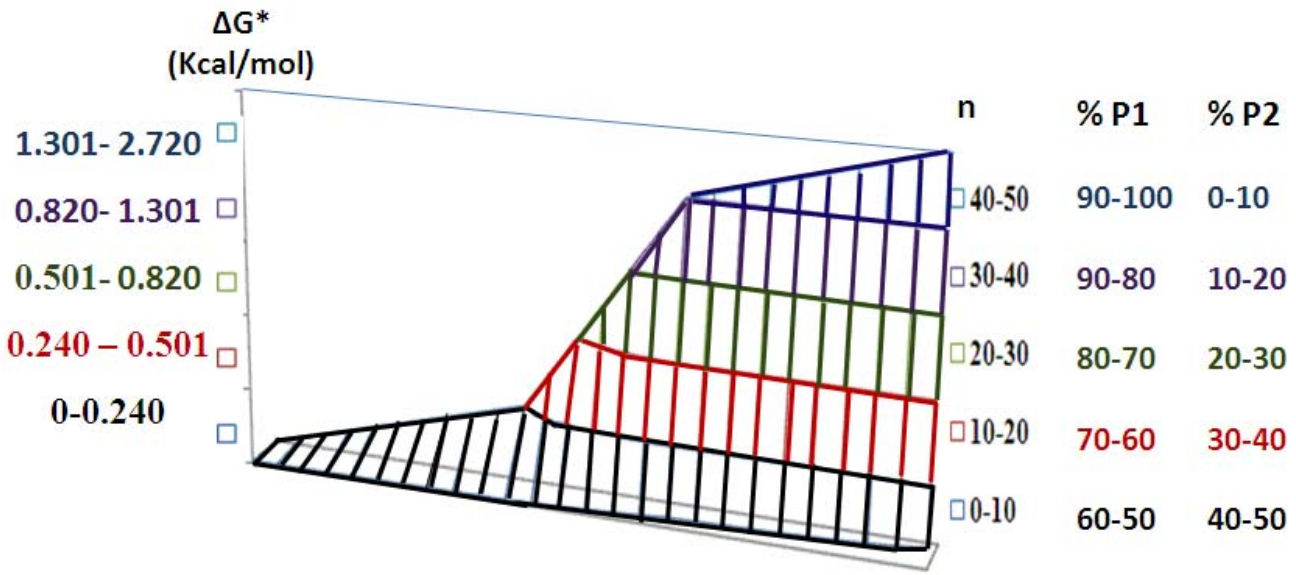


Figure 4: $\Delta G^{\#}(P2) - \Delta G^{\#}(P1)$ Difference of relative free energy (in Kcal/mol) and percentage of the products

We can deduce from figure 4 that:

- When $\Delta G^{\#}(P2) - \Delta G^{\#}(P1) = 0$, n=0, consequently the percentages of the products are equal (%P_1=%P_2= 50%).
- When $\Delta G^{\#}(P2) - \Delta G^{\#}(P1)$ varies between 0 and 0.240 (eV), n varies between 0 and 10, therefore the reaction will be selective (regio, sterio, diasterio and chemio) and the percentages of P_1 varies between] 50 - 60] and the percentages of P_2 varies between] 40 - 50[.
- When $\Delta G^{\#}(P2) - \Delta G^{\#}(P1)$ takes values between 1.301-2.720 (eV), n varies between 40-50, the percentages of the product P1 varies between] 90 - 100[and the percentages of the product P2 varies

between]0-10[, consequently the reaction will be very selective.

- When $\Delta G^{\#}(P2) - \Delta G^{\#}(P1)$ is greater than 2.720 (eV) the reaction will be specific (%P1= 100%)
- In this work we observed that the difference of relative free energy are superior than 2.720 (eV), indicated that these reactions are regio-specific in good agreement with experimental result.

IV. Conclusion

In this paper, we have discussed the molecular mechanism and the regioselectivity of the [1+2] cycloaddition reactions of limonene **1**, terpinolene **2** and γ-terpinene **3.** with dichlorocarbene yielding 1a, 2a and 3a, respectively, experimentally studied by by Hossni Ziyat et al, has been investigated using DFT methods at the DFT/6-31G(d,p) computational level. Analysis of the nucleophilic P_k^- Parr functions allows characterising the carbons atoms of the double multi-substitute as the most nucleophilic centre of the monoterpenes (limonene **1**, terpinolene **2** and γ-terpinene **3**) used in this work, in clear agreement with the regioselectivity found in result. An exploration of the PESs associated with these cycloaddition reactions indicates that these cycloaddition reactions are strongly exothermic, and from the activation free energies we can conclude that these reactions are completely regiospecific.

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Voltammetric Determination of Bromethalin by using Polymer Coated Ion Selective Bare Carbon Electrode

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Keywords: bromethalin, differential pulse adsorptive stripping voltametric method, polymer coated ion selective electrode, universal buffer solution.

GJSFR-B Classification: FOR Code: 030305

Strictly as per the compliance and regulations of :

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Sekharreddy S. R [α], T. R. Babu [σ], P. Sreeharireddy [ρ] & J. Subrahmanyam [ω]

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I. Introduction

Bromethalin [α,α,α-trifluoro-N-methyl-4,6-dinitro-N-(2,4,6-tribromophenyl)-o-toluidine] is a new commercial dinitroaniline rodenticide for the control of comensal rodents. Current methods for the analysis of pesticides containing nitro group compounds involve either liquid –liquid extraction [1] solid-phase extraction (SPE)[2] supercritical fluid extraction (SCFE) and solid phase micro extraction (SPME) [3].The main disadvantages of these methods were use of large quantities are often toxic and not eco-friendly solvents, the elaborate cleaning up time-consuming procedures and the need for concentration of analytes before analysis [4]. Mesmer and Fluler [5] reported high performance liquid chromatography with UV-VIS spectrometric and HPLC negative-ion. Braselten and Jonson [6] reported TLC extended by GC/MS to determine bromethalin in environmental samples. Melissa et al [7] developed a new type of all-solid-state ion-selective electrode based on a transuding layer of a network of single-walled carbon nanotubes. The extraordinary capacity of carbon nanotubes to promote electron transfer between heterogeneous phases made the presence of electroactive polymers or any other ion-to-electron-transfer promoter. Javad Zolgharnein et al. [8] reported simultaneous determination of propanil and monalide by modified glassy carbon electrode with nickel oxide nanoparticles, using partial least squares modified by orthogonal signal correction and wavelet packet transform.Though metal and non metal electrodes used for electro analysis [9-10] better reproducibility achieved in this approach.

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II. Experimental

a) Apparatus and Electrodes

The electrochemical measurements were carried out with Metrohm model 101 potentiostat and galvanostat. The three-electrode system consisted of polymer coated ion selective bare carbon electrode prepared by using poly vinyl chloride (PVC) solvent membrane and tetra phenyl borate(TPB) as ion pairing agent used as working electrode. Ag/AgCl reference electrode and a platinum wire used as auxiliary electrode. The electrodes joined the cell through holes in its Teflon cover. All of the potentials given in this work were measured with respect to this reference system. Electrochemical experiments were carried out in a voltametric cell at room temperature. A magnetic stirrer was used during the accumulation step. The Eli co Li-129 model glass calomel combined electrode was employed for measuring pH values.

b) Reagents and solutions

All reagents used were of analytical reagent grade. Double distilled water is used throughout the analysis. In the present investigation, universal buffers in the pH range 2.0 to 6.0 are used as supporting electrolytes and prepared using 0.2 M boric acid, 0.05 M citric acid and 0.1 M tri sodium orthophosphate solutions. Pesticide samples are obtained from Bayer crop, India, Ltd.

III. Result and Discussion

Bromethalin is found to a give a single well defined peak in acidic solutions (2 < pH < 6). Increase of pH from 4.0 leads to decrease of the peak current. In the acidic medium, the peak of the compound is due to the reduction of 2 nitro groups in 4 electron process. Typical cyclic voltammogram shown in Fig.1.

The reduction process of bromethalin is found to be diffusion controlled and adsorption on the electrode surface in the buffer systems studied as evidenced from linear plot $i_p$vs $v^{1/2}$ passing through origin. The shift of peak potential (E_p) towards more negative values with increase in concentration of depolarizer, shows that the electrode process is irreversible. This is further confirmed by log-plot analysis. The variation of peak potentials with scan rates and absence of anodic peak in the reverse scan in cyclic voltammetry indicates the irreversible nature of the electrode processes. The dependence of i_p/pH curves shows a behavior in accordance with a process in which a proton transfer provides the reduction of the acid form to form an electro active species. The number of protons taking part in the rate determining step is 4.

Millicoulometry is employed to find out the number of electrons involved in the electrode process. The results obtained from millicoulometry have shown that the number of electrons is 4 for bromethalin. The number of protons involved in the rate determining step (scheme I) of the electrode process is 4. Controlled potential electrolysis experiments are carried out at -0.8 V at saturated colomel electrode at pH 4.0.to collect reduction product.

Kinetic data such as diffusion coefficient, transfer coefficient and heterogeneous forward rate constants obtained for bromethalin is summarized in table 1.0.The diffusion coefficient values are noticed to be in good agreement from cyclic voltammetry. The heterogeneous forward rate constants were decreasing with an increase in pH of the supporting electrolyte, which may responsible for the shift of reduction potentials towards more negative values with increase in pH. This trend is particularly evident where the proton transfer is involved in the electrode process.

a) Dp-ASV studies and optimum conditions

Peak of bromethalin at working electrode (Fig.2.0) is attributed to reduction of bromethalin.This peak followed to establish the optimum conditions. The standard addition and calibration methods have been employed to estimate the compound in grain samples. Maximum peak potentials are obtained with pH 4.0.The shift of the peak potentials towards more negative values indicating proton participation in the reduction process.

The effects of varying the potential scan rate on the reduction peak current of bromethalin is examined. The reduction peak current increases linearly with scan rate over the range from 20 mVs^{-1} to 60 mVs^{-1} as expected for the reduction of being observed. Best sensitivity achieved at a scan rate of 50 mVs^{-1}.

IV. Recovery Experiments

a) Analysis

Well defined and well resolved AdSV peaks of bromethalin obtained at pH 4.0 is used for the quantitative estimation of bromethalin in water and soil samples. Both calibration and standard addition methods are used for the quantitative determination of bromethalin. From the calibration method, it is observed that the peak current shows a trend found to be linear over the concentration range Peak currents were linear over the concentration range of 1.4x 10^{-8} M to 1.3×10^{-9} M with lower detection limit of 10^{-10} M. The relative standard deviation and correlation coefficients are found to be 1.15%, 0.985 respectively for 10 replicates. Calculations made by standard addition method.

b) Recommended analytical procedure

The stock solution (1.0 x 10^{-5} M) of bromethalin is prepared by dissolving the required quantity of the electroactive species in methanol. Standard solutions are prepared by dilution of stock solution with suitable amount of methanol. 1 mL of the standard solution is transferred into voltammetric cell and added with 9 mL of the supporting electrolyte and then deoxygenated by bubbling oxygen free nitrogen gas for 10 min. After recording the voltammogram, small increments of standard solutions (0.2 mL) added and then voltammograms recorded for each addition under similar experimental conditions. The optimum conditions for the analytical determination of bromethalin are pH 4.0 and scan rate 50 mVs^{-1}.

c) Determination of bromethalin in spiked grain samples

The developed analytical procedure has been applied to the quantitative estimation bromethalin in grain samples. Known amount of bromethalin is sprayed on grain samples (25 g) and left for 1-2 hours. Then the samples are weighed, crushed and homogenized and treated with 50mL acetone and evaporated to dryness. The residue of bromethalin dissolved in methanol and transferred to a 100 mL volumetric flask. 1 mL of the standard solution is transferred into voltammetric cell and added with 9 mL of the supporting electrolyte and then deoxygenated by bubbling oxygen free nitrogen gas for 10 min. After recording the voltammogram, small increments of standard solutions (0.2 mL) were added and then voltammograms recorded for each addition under similar experimental conditions. Results obtained for the determination of bromethalin in grains by this method ranged from 98.66 to 99.50% which indicates

the high accuracy and reproducibility of the proposed method. The results are summarized in table.2.0

V. Conclusion

The present part describes the detailed study of electrochemical reduction of nitro group containing pesticide bromethalin from the results obtained from cyclic voltammetry, differential pulse adsorptive stripping voltammetry, millicoulometry and controlled potential electrolysis in methanol as solvent in the supporting electrolytes of pH ranging 2.0 to 6.0. To overcome partial load over current density and for improved electrode kinetics polymer coated ion selective bare carbon electrode prepared by using poly vinyl chloride (PVC) solvent membrane and tetra phenyl borate (TPB) as ion pairing agent used as working electrode to avoid the environmental pollution arises due to metal electrodes.

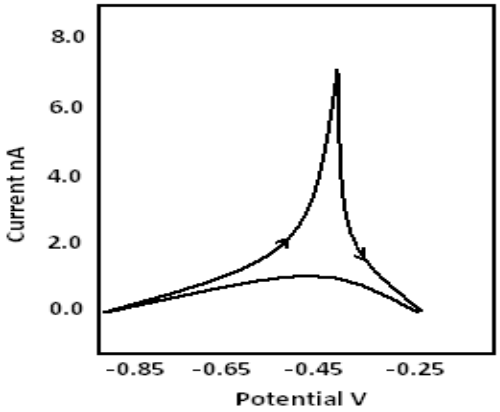


Fig.1.0: Typical cyclic voltammogram of bromethalin at polymer membrane electrode, pH 4.0 concentration: 0.5 mM; scan rate: 50 mVs^{-1}

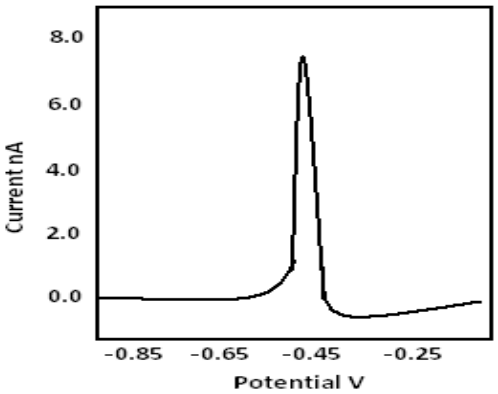
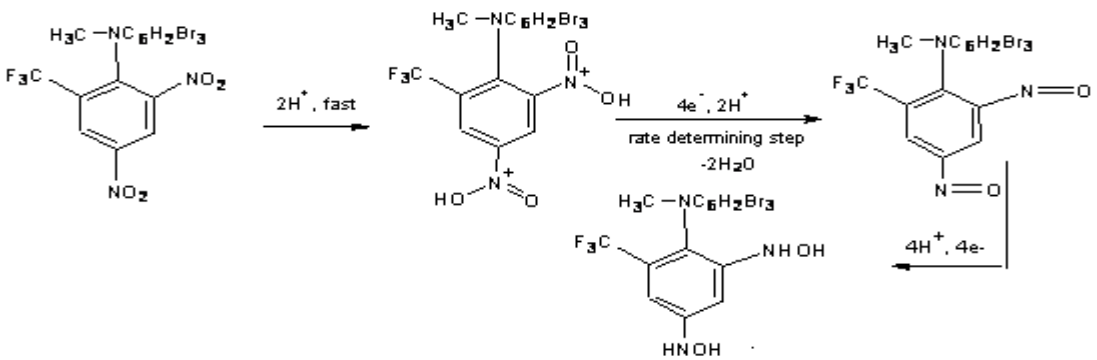


Fig. 2.0: Typical differential pulse adsorptive stripping voltammogram of bromethalin at polymer membrane electrode, pH4.0, scan rate: 50mVs^{-1}



Scheme I: Reduction mechanism of bromethalin at polymer membrane electrode: pH 4.0.

Table 1: Typical cyclic voltammetric data of of bromethalin:concentration: 0.5 mM, scan rate: 50mVs^{-1}

pH	Ep/V	Ip/nA	$\alpha\, n_a$	$\frac{D \times 10^6}{cm^2\ s^{-1}}$	$\frac{k^0_{f,h}}{cm\ s^{-1}}$
4.0	0.45	6.5	0.42	1.28	1.02 x 10^{-10}

Table 2: Recoveries of of bromethalin in spiked grain samples

Grains	Amount added (ng/mL)	Amount found (ng/mL)	Recovery (%)	Standard deviation
Black gram	2.0	1.99	99.50	0.021
Rice	3.0	2.96	98.66	0.007

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Application of DPP for the Determination of Cefdinir in Pharmaceuticals

By Salam A.H. Al-Ameri
Al-Mustansiriyha University

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The linear range was recognized between 0.875- 7.000 $\mu g.ml^{-1}$. The calculated results show that LOD and LOQ were equals to 0.3271and 1.0904 $\mu g.ml^{-1}$ respectively. This method was successfully applied to assay cefdinir in commercial capsules with 0.089 standard deviation and relative standard deviation less than 2.97 %. The proposed method is simple, accurate, fewer time consuming and even applied without prior separation for the color and excipient solution.

Keywords: *Cefdinir; DPP; KNO_3; LiCl.*

GJSFR-B Classification: *FOR Code: 030599*

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I. Introduction

Cefdinir is a extremely beta-lactamase stable third-generation cephalosporin that need been concurred for those medication of a few type of bacterial diseases, chemically known as [(6R,7R)-7-[[(2Z)-(2-amino4-thiazolyl)(hydroxylimino) acetyl]amino]-3-ethenyl-8-oxo-5- thia-1-azabicyclo [4.2.0]oct-2-ene-2-carboxylic acid] ,Figure 1[1, 2].

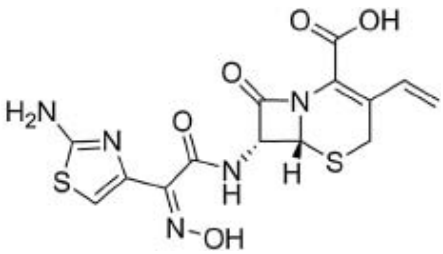

Fig. 1: Chemical structure of Cefdinir

DPP technique was applied for estimation a number of drugs as quality control [3]. Several analytical needs been describe for those assurance of cefdinir to pharmaceuticals what's all the more living samples. Cefdinir oxidation and reduction voltammetric behavior was studied using hanging mercury dropping electrode HMDE, and glassy carbon electrode GCE versus Ag/AgCl at pH 4.2 and 5.0 respectively, also a developed adsorptive stripping voltammetric method for cefdinir assay in diverse samples. The results illustrate that linear range among 0.25 to 0.4 µM for HMDE and 0.4 to 10 µM for GCE and the LOQ was 0.2 and 0.26 µM for HMDE and GCE respectively [1].

Direct current polarography, differential pulse polarography and cyclic voltammetry was applied for the cefdinir electrochemical behavior studying at pH ranged from 2 – 12. Diffusion coefficient, transfer coefficient and rate constant as kinetic parameters were calculated. Also the method used for the drug estimation in pharmaceuticals and life tasters [2].

New developed spectrophotometric methods for the cefdinir assay in pure sample and pharmaceuticals, in the first, an orange colored complex formed between cefdinir and NQS reagent at pH 11 which analysis at 490 nm while in the second method a yellow colored complex formed between hydrolysis cefdinir with NBD-Cl reagent which analysis at 390 nm. The results show satisfactory accuracy and precision [4].

A developed first derivative spectrophotometric technique was applied for the assay of cefdinir and cefixime in pharmaceuticals using $NaHPO_4$ at alkaline solution, pH=8, which measured at 306.8 nm. The results show LOD values was 0.28; 0.45 µg/ml and LOQ value was 0.98; 1.5 µg/ml for cefdinir and cefixime.respectively [5].

This study was meant to develop sensitive and simple polarographic method for direct estimation of cefdinir in pharmaceuticals, In addition to, it was intended to examine the reduction behavior of cefdinir on DME electrode, also uncertain reaction mechanisms were proposed.

II. Experimental

a) Apparatus

All polarographic analyses were done with a 797VA Computrace, Metrohom, Herisau, Switzerland which including the three-electrode mode consisted of Dropping Mercury Electrode, DME as working electrode, Ag/AgCl; 3 M KCl as a reference electrode and a Pt auxiliary electrode. pH measurements were get using HANNA pH 211, Microprocessor pH meter, Romania. Distilled water used was obtained from a Water still W4000, Merit. The measurements were carrying out at room temperature ± 5°C.

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b) Materials and reagents

Every chemicals used were of analytical mark purity and used without additional purification. All the standard, reagents and sample solutions were prepared using distilled water. The cefdinir standard was purchased from Astellas Pharma Inc. Tokyo, Japan. The cefdinir stock solutions (1000 μg.ml^{-1}) were prepared in D.W and stored at less than 4° C. All cefdinir sample solutions were prepared by enough dilution of stock solution. A Sefarin 300mg, pharma international co., Amman, Jordan was selected as commercial pharmaceuticals.

c) Procedure

An aliquot volume of cefdinir sample solutions was pour into a 20 ml polarographic cell. The voltammetric analyses were carried out after degassing the cell with high purity nitrogen for 5 minutes and then analysis by scanning the potential within the negative direction on DME as working electrode versus Ag/AgCl, 3.0 M KCl as reference electrode and platinum wire as an auxiliary electrode. The final volume in the polarographic cell with all solutions added, cefdinir sample, 0.2 to 0.4ml volume of 3M KNO_3 or 0.5M LiCl as a supporting electrolyte and 2ml Briton-Robinson buffers [6, 7] solutions were completed to the 20 ml with distilled water as a solvent, Table-1.

Table-1: The optimum experimental parameters established for cefdinir analysis

Parameters	Conditions value	Parameters	Conditions value
Working electrode	DME	Initial potential	0.00 mV
Supporting electrolyte	KNO_3 or LiCl	Final potential	-1.8 mV
Buffer	B-R, pH 4 and 7	Pulse amplitude	50 mV
Purge gas	99.999% Purity nitrogen	Scan rate	5 mV/sec
Purge time	300 sec	Peak potential	- 0.360 to -0.710 V

d) Preparation of commercial Cefdinir

Cefdinir 300mg capsules were get from a local pharmacy in Baghdad and used as a dosage form. Two capsules each one contains 300 mg cefdinir were mixed well and homogeneous then an accurate weighed sample was transferred into a 50 ml volumetric flask containing 10 ml of distilled water. The solution inside the volumetric flask were shakes severely for few minutes and the volume of this flask was completed to the total volume using D.W, then this solution was filtered and the clear solution was used to prepare the like concentration for the analysis.

III. Results & Discussion

a) pH effect

The DPP reduction polarogram of cefdinir at the optimal experimental conditions showed one clear and more sensitive reduction peak at applied potential ranging from -0.5 to – 0.95 V with other slight sensitive peaks.

The peak current of cefdinir at pH values, 4, 7 and 9 showed more negative E ½ voltage when the acidity lessen, Figure 2, therefore, at the alkaline solution, a little proton ion involvement, the reduction process isn't simply facilitate compared with neutral and acidic media, [8, 9] also the results show an relative decreasing in the peak intensity and sensitivity in alkaline media, this results confirm that the reduction reaction engage the protons and the cefdinir electrochemical activities depends on the pH.

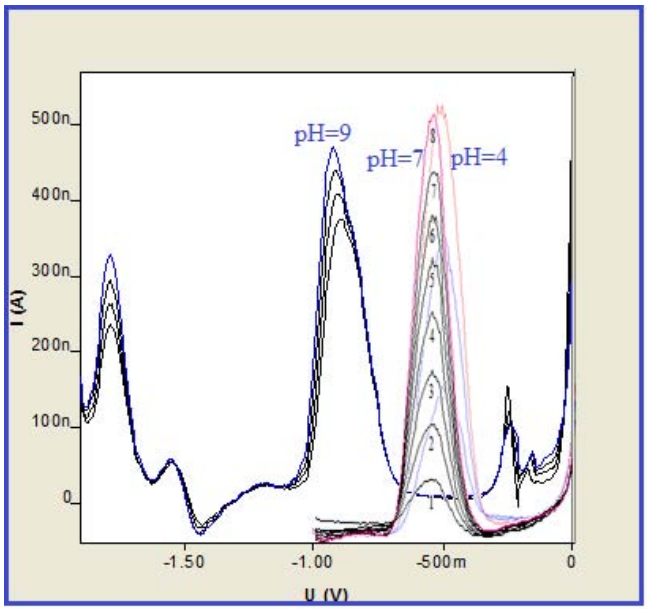

Figure 2: DPP polarograms for cefdinir solutions at pH 4,7 and 9

b) Calibration plot

For the determination of cefdinir, a standard calibration plot of cefdinir was prepared and applied using the Least Squares Method, LSM [10] in the concentration range 0.875-7.000 μg.ml^{-1} using DPP on DME in Britton-Robinson buffer at pH 4 and 7 also 0.06M KNO_3 and 0.01M LiCl. One reduction peak has height greatness and sensitivity in – 0.518v was observed and chooses. The peak current ip was proportional to the concentration, Figs.3 and 4. The accuracy and precision of the method was tested, the

results showed the SD was 2.14 and LOD and LOQ was 0.3271 and 1.09 μg.ml^{-1} respectively, the regression equation and correlation coefficient, r, and other analytical merit number [10] were summarized in Table-2.

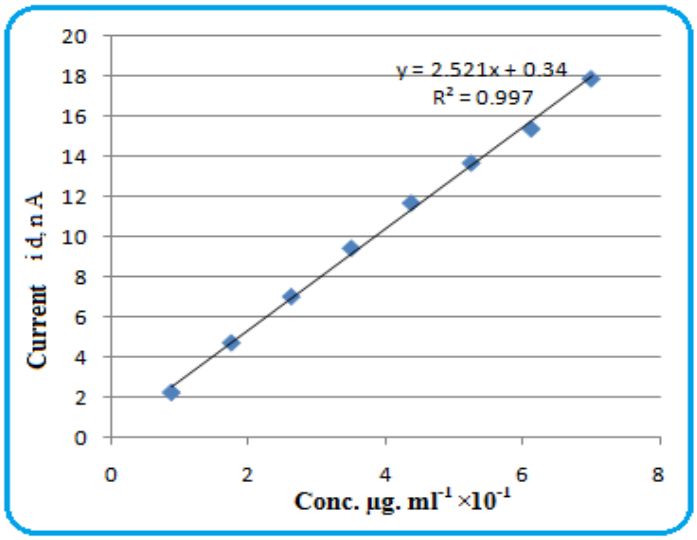

Figure 3: Calibration curves for the determination of cefdinir using DPP at optimal conditions

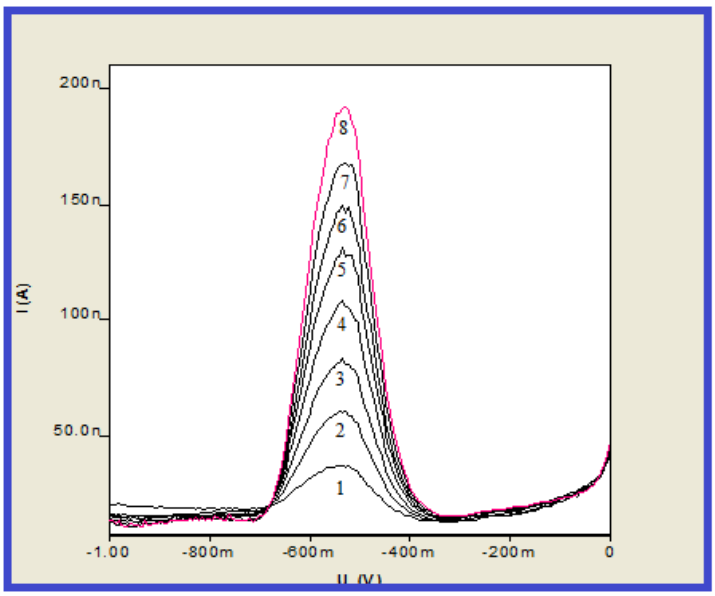

Figure 4: The DPP polarograms of cefdinir at optimum conditions in pH= 4 and B-R buffer at concentrations range 0.875 to 7.0 µg.ml^{-1}

Table-2: Analytical merit number for the assaying of cefidinr by suggested DPP method

Parameters	Values	Parameters	Values
Regression equation	id = 2.521 X + 0.34	Random errors in the Y direction, $S_{y/x}$	0.2749
Concentration range, μg.ml^{-1}	0.875 to 7.000	Standard deviation of slope, S_b	0.0485
Slope of the line, b	2.521	Standard deviation of intercept, S_a	0.214
Intercept, a	+ 0.34	C.L. for the slope (b ± $t_{(n-2)}$ S_b) at 95%	2.521 ± 0.1188
Correlation coefficient, r	0.9984	C.L. for the intercept (a± $t_{(n-2)}$Sa) at 95%	0.34 ± 0.524
Coefficient of determination, R^2	0.9968	LOD 3.3 SD, μg.ml^{-1}	0.3271
Standard deviation, SD	2.14	LOQ 10 SD, μg.ml^{-1}	1.09

c) Applications

The accuracy, precision and repeatability of the method was experienced by deference measurements for 3 and 5 μg.ml^{-1} synthetic cefdinir samples, the amounts found to be 3.06 ± 0.13 and 5.09± 0.23 and the relative error ranged between -1 to +4.3 and -0.98 to

+4.52, also the results show suitable and accurate values for standard error of the mean and the confidence limit of the mean, Table-3.

Table-3: Determination of cefdinir in synthetic sample in B-R buffer at pH 4

Initial Conc. µg.ml^{-1}	Calculated Conc., av. µg.ml^{-1}	SD	RSD	Absolute Error, Range	%Relative Error	Standard Error of the mean	Confidence limit of the mean
3.00	3.06	0.089	2.97	-0.03 to +0.13	-1 to +4.3	0.036	3.06 ± 0.0934
5.00	5.09	0.13	2.55	-0.08 to +0.23	-0.98 to +4.52	0.32	5.09 ± 0.136

n=6, t= 2.57

The application for the cefdinir determination in commercial pharmaceuticals using DPP on DME in B-R buffer at pH 4 in 0.06M KNO_3 or 0.01M LiCl, the result shows that the absolute error ranged within the 0.08 to +0.17 and the relative error don't exceed 2.8%, Table-4, the results prove that method has accepted precision and repeatability.

Table-4: Determination of cefdinir in pharmaceutical sample in B-R buffer at pH 4

Initial Conc. µg.ml^{-1}	Calculated Conc., av. µg.ml^{-1}	SD	RSD	Absolute Error, Range	%Relative Error	Standard Error of the mean	Confidence limit of the mean
6.00	6.11	0.1	1.62	-0.08 to +0.17	-1.3 to + 2.8	0.045	6.11± 0.124

n=5, t=2.78

e) Electro-chemical activities and number of electrons

The ilkovic-Heyrovsky equation describes the entire current – potential curve and calculates the number of shared electrons in the electrode process of a reversible redox system in polarography.

$$E = E_{1/2} + \frac{RT}{nF} \ln\left(\frac{i_d - i}{i}\right)$$

Where id is the diffusion current and i is the current at these points of the polarographic stage which corresponding to the applied potential E, and E ½ is the half-Wave potential, [8, 9, 11] hence by plotting applied potential, E against log{(i-id) / i}, a straight line is obtained which present that the electrode process is reversible in these case that the slope of the line indicated the values of n, i.e. the number of electrons transferred in the electrode reaction in view to the wave reversibility, when the number of electrons was integers numbers, it's refers to reversible electrochemical process, whereas the rational number refers to irreversible electrochemical process [12, 13].The calculated value of the E ½ was -0.504V and 4 electrons really required for the reduction, Figure 5, thereby, depending on the number of electrons obtained and $E_{1/2}$, the choicest planned reduction mechanism recommended that the azomethine group gets reduce to the saturated amine group via actually four electrons process at reversible electrochemical process, this reduction takes place at neutral and alkaline solution and at about -0.4v, reaction A, while the preferred reduction mechanism in acidic solution recommended reduce the azomethine group to the ammonium ion, reaction B, owing to the presence concentration of protons participation appear to make the reduction easier allowed to form ammonium salt, Figure 6 [8, 14].

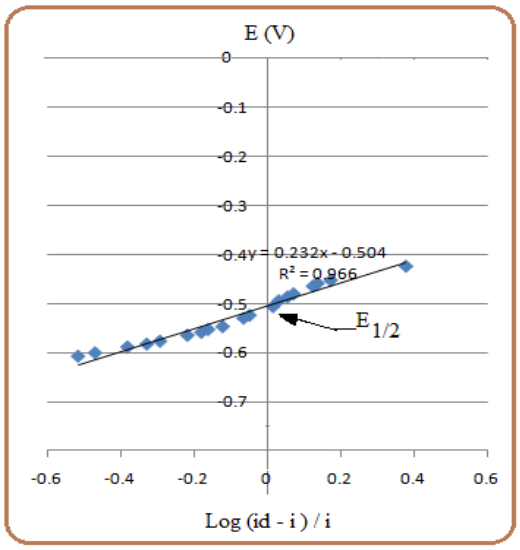

Figure 5: The relation between the potential E and the logarithms of { (i-id) / i }for cefdinir

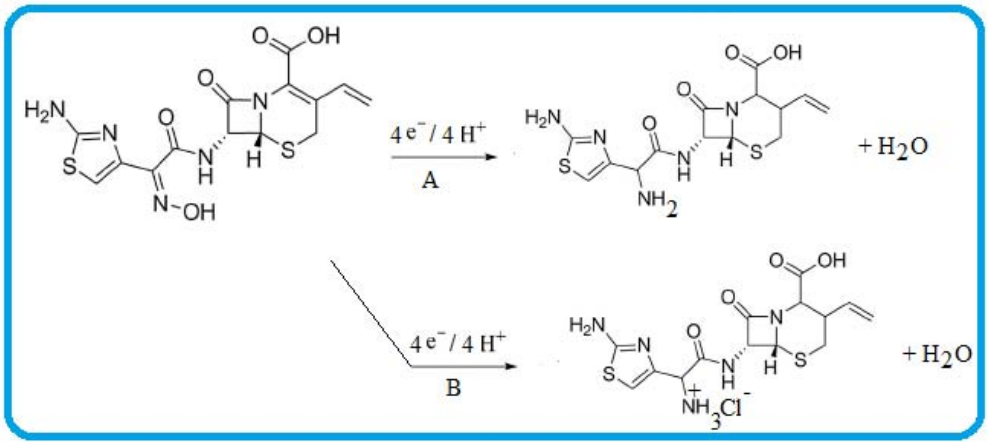

Figure 6: Optional and expect reduction mechanism of cefdinir

IV. Conclusion

The electo-chemical reduction activities and analysis of the cefdinir drug in B-R buffer over a pH range of 4-9 was studied. The participation proton appear to make the reduction easier, other than in basic media, the reduction route isn't make easy due to the non- availability of protons [12]. The statistics results confirm that DPP is one of the finest analytical apparatus for drugs estimations, more, this technique is sensitive, accurate and needed a fewer time also, it's used without prior separation for color and excipient samples before the analysis.

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3. Submission of Manuscripts,

4. Manuscript's Category,

5. Structure and Format of Manuscript,

6. After Acceptance.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Informal Guidelines of Research Paper Writing

Key points to remember:

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

Final Points:

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

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

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

General style:

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

To make a paper clear

· Adhere to recommended page limits

Mistakes to evade

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

In every sections of your document

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

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

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

· Align the primary line of each section

· Present your points in sound order

· Use present tense to report well accepted

· Use past tense to describe specific results

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

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

Title Page:

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

Abstract:

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

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

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

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

Approach:

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

Introduction:

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

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

Approach:

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

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

Procedures (Methods and Materials):

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

Materials:

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

Methods:

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

Approach:

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

What to keep away from

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

Results:

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

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

Content

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

What to stay away from

- Do not discuss or infer your outcome, report surroundings information, or try to explain anything.
- Not at all, take in raw data or intermediate calculations in a research manuscript.
- Do not present the similar data more than once.
- Manuscript should complement any figures or tables, not duplicate the identical information.
- Never confuse figures with tables - there is a difference.

Approach

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

Figures and tables

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

Discussion:

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

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

Approach:

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

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

Segment Draft and Final Research Paper: You have to strictly follow the template of research paper. If it is not done your paper may get rejected.

- The **major constraint** is that you must independently make all content, tables, graphs, and facts that are offered in the paper. You must write each part of the paper wholly on your own. The Peer-reviewers need to identify your own perceptive of the concepts in your own terms. NEVER extract straight from any foundation, and never rephrase someone else's analysis.

- Do not give permission to anyone else to "PROOFREAD" your manuscript.

- Methods to avoid Plagiarism is applied by us on every paper, if found guilty, you will be blacklisted by all of our collaborated research groups, your institution will be informed for this and strict legal actions will be taken immediately.)
- To guard yourself and others from possible illegal use please do not permit anyone right to use to your paper and files.

Criterion for Grading a Research Paper (Compilation) by Global Journals Inc. (US)

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

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