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KINETICS OF HETEROCYCLIC COMPOUND

***B.Y. Pagare*[1,*], *A.B. Gambhire*[1], *S.P. Lawande*[2], *B.R. Arbad*[3]**

[1]Department of Chemistry, Shri Anand College, Pathardi, 414102, Dist. Ahmednagar, MS, India
[2]Department of Chemistry, Shri Chhatrapati Shivaji Mahavidyalaya, Shrigonda, Ahmednagar, MS, India
[3]Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, 431004. MS, India

***Corresponding author email:** byp_chem@ymail.com

ABSTRACT: Kinetics of heterocyclic compound has been studied. Formation of 4-thiazolidinone reaction follows overall second order kinetics. Schiff base and thioacid reaction is catalyzed by toluene-4-sulphonic acid and kinetic measurements are obtained. The influence of dielectric constant on a rate of reaction has been studied.

KEYWORDS: Schiff bases, Thiolactic Acid, 4-thiazolidinone, toluene-4-sulfonic acid, Galacial acetic acid, Formic acid.

1. INTRODUCTION

Schiff bases are used in synthesis of thiazolidinone [1]. Thiolactic acid is used as cyclisation agent in synthesis of 4-thiazolidinone [2]. 4-thiazolidinone and its derivative exhibit variety of pharmacological activities [3-6]. In view of the wide applications associated with 4-thiazolidinone, the attempts have been made to investigate the kinetics of this reaction. The present research work deals with kinetic study of 4-thiazolidinone heterocyclic compound under the influence of solvent effect in presence of tolunene-4-sulphonic acid as a catalyst.

2. EXPERIMENTAL

TLA (A. R. Fluka, 97 % purity) solutions were standardized by using standard solution of iodine (A. R. Grade) [7]. Various SB were prepared in suitable solvents. P-TSA (A. R. Grade, Merk) was used as a catalyst. Kinetic experiments were carried out in a thermostatic water-bath in chloroform/acetic acid medium at temperature 303.15, 308.15, 313.15 and 318.15 °K. The reaction was followed by withdrawing aliquots of reaction mixture at interval of time and estimating the reacted TLA idiomatically. The formation of product 4-thiazolidinone was confirmed by IR, NMR spectra and elemental analysis. In present study, kinetic measurements were carried out at various dielectric constants of the medium by using different mix composition of acetic acid and formic acid.

3. RESULTS AND DISCUSSION

The second order rate constant (k) determined at different concentration of SB and TLA vice-versa and observed nearly constant suggest that the overall reaction follows second order kinetics. Scatchard [8] gave a quantitative estimate of the effect of dielectric constant of the medium.

In present work, the rate of reaction increases with increasing dielectric constant of the medium, which supports the presence of ion-ion type reaction. While increase in the rate of reaction with decrease in dielectric constant of the medium support the presence of ion-dipole type of reaction [9-12]. The rate of Cyclocondensation reaction increases with increase in the dielectric constant of the medium. This may be due to the development of change in the transition state of the reaction and also due to increase in the ionizing power of the medium [13, 14]. The increase in rate with an increase in polarity of the medium suggests that the transition state of the rate determining step is more polar than the reactants. The solvent effect can also be analysed using Grunwald-Winstein equation [15-16]. In the present study d A-B values for four representative components (A1,B1,C1 and D1 were calculated from the slope of the plot log k versus 1/D [17-20].

Table 1. Variation of [SB] at constant [TLA], [p-TSA] and Temperature**.**
[TLA] = 0.05M, [p-TSA] = 300 mgs, Temp = 303°K, Solvent = Chloroform

Sr.No.	[SB] M	$k \times 10^3$ By calculation	$k \times 10^3$ By graphical
1	0.05	3.513	3.533
2	0.04	3.485	3.403
3	0.03	3.428	3.454
4	0.02	3.397	3.300
5	0.01	3.171	3.166

Table 2. Variation of [TLA] at constant [SB], [p-TSA] and Temperature.

Sr.No.	[SB] M	$k \times 10^3$ By calculation	$k \times 10^3$ By graphical
1	0.05	3.513	3.522
2	0.04	3.485	3.403
3	0.03	3.471	3.467
4	0.02	3.454	3.420
5	0.01	3.440	3.345

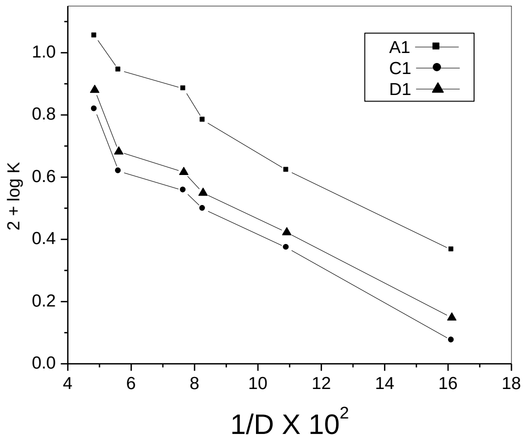

Fig. 1. 2 + log k v/s (1/D) × 10^2

4. Conclusions

The rate of reaction is directly proportional to the dielectric constant of the medium which indicates the presence of ion-ion type reaction.

Table 3. Effect of variation of Dielectric Constant [SB] = 0.02M, [TLA] = 0.02M, Temp = 303 o K, Solvent = Acetic acid + Formic acid, [p-TSA] = 0.0525mgs.

Sr.No.	D	$1/D \times 10^2$	$k \times 10^2$	2+logk	$k \times 10^2$	2+logk	$k \times 10^2$	2+logk
1	6.20	16.12	2.328	0.366	1.190	0.075	1.408	0.148
2	9.16	10.91	4.194	0.622	2.363	0.373	2.660	0.422
3	12.09	8.27	6.072	0.783	3.148	0.498	3.545	0.549
4	14.98	7.66	7.668	0.884	3.610	0.557	4.134	0.616
5	17.82	5.61	8.808	0.944	4.163	0.619	4.818	0.682
6	20.63	4.85	11.33	1.054	6.591	0.818	6.900	0.880

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