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A STUDY OF SOLVENT EFFECTS ON THE REACTION BETWEEN p-NITROBENZYL CHLORIDE AND HYDROXIDE ION IN AQUEOUS DIOXANE HOMOGENEOUS MEDIA

BY

KEN K. HO, [illegible]

A

THESIS

submitted to the faculty of

THE UNIVERSITY OF MISSOURI - ROLLA

in partial fulfillment of the requirements for the

Degree of

MASTER OF SCIENCE IN CHEMISTRY

Rolla, Missouri

1968

134385

Approved by

[signature] (advisor) [signature]

[signature]

ACKNOWLEDGEMENT

We Chinese are supposed to be born philosophers and poets but now I am lost for words.

To Dr. Samir B. Hanna goes my gratitude for his invaluable advice, persuasive encouragement and endless patience through out my period of study here at Rolla to make this investigation possible and especially at the time of preparation of this manuscript just before his one-year travelling to Switzerland.

My appreciation goes to Dr. Raymond L. Venable for the timely help, and advice with kindly consideration when all seemed to be lost.

And last but not least, I salute all those who made my stay here in Rolla so rewarding - special thanks to you all.

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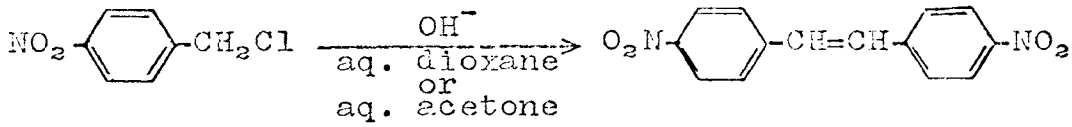
ABSTRACT

The kinetics and activation parameters of the reaction between p-nitrobenzyl chloride and hydroxide ion, leading to the formation of p, p'- dinitrostilbene quantitatively, have been studied in five aqueous dioxane solvent systems at five different temperatures between 20° and 40°C. At any one temperature the second-order rate constants are minimum in the 30% dioxane solvent mixture, reach a maximum in the 50% dioxane systems, and fall off slightly in the 60% and 70% dioxane systems. The Arrhenius activation energies are highest in the 30% dioxane and lowest in the 70% dioxane systems. The free energies of activation change in the same direction but the magnitude of change is much less than that for E_a or ΔH^*. The greatest variation is shown in the entropies of activation: 14.4 e.u. in the 30% aqueous dioxane solvent mixture and only 2.5 e.u. in the 70% system. The significance of these results is discussed in terms of specific solute-solvent interactions, dielectric constants, and variations in the activities of hydroxide ion with variations in the solvent composition.

I. INTRODUCTION

p-Nitrobenzyl chloride is a peculiarly reactive halide. Its behavior in alkaline aqueous aprotic solvent mixtures is basically different from the behavior of all other substituted benzyl halides studied in the same media to date[1]. Instead of the usually observed hydrolysis, p-nitrobenzyl chloride undergoes an eliminative condensation to p,p'-dinitrostilbene in quantitative yield in the said media[1].



The kinetics of this reaction has been reported[1], and despite the controversies about the details of the possible mechanisms[2-4], the most accepted mechanism is the following[1]:

---

1. Hanna, S. B., Iskander, Y., and Riad, Y.
J. Chem. Soc., 217, 221 (1961)

2. Swain, C. G. and Thornton, E. R.
J. Am. Chem. Soc., 83, 4033 (1961)

3. Hartzler, H. D.
J. Am. Chem. Soc., 83, 4997 (1961)

4. Hine, J.
"Divalent Carbon"
The Ronald Press Company, New York, Chapter 6 (1964)

(1) $Ar\text{-}CH_2\text{-}Cl + OH^- \underset{\text{equilibrium*}}{\overset{\text{fast}}{\rightleftharpoons}} Ar\bar{C}H\text{-}Cl + H_2O$

(2) $Ar\text{-}\bar{C}H\text{-}Cl \xrightarrow[\text{step}]{\text{rate-determining}} Ar\text{-}CH: + Cl^-$

(3) $2\ Ar\text{-}CH: \xrightarrow{\text{dimerization}} Ar\text{-}CH{=}CH\text{-}Ar$

(3') or $Ar\text{-}CH: + Ar\text{-}\bar{C}H\text{-}Cl \xrightarrow{\text{fast}} Ar\text{-}CH{=}CH\text{-}Ar + Cl^-$

The proposed rate-determining step finds parallelism in the much-studied Hofmann and Lossen rearrangements of compounds of the type R-CO-NHX in the presence of alkalis[5].

In recent years much attention has been given to the study of the solvolysis of benzyl chloride in mixed solvents[6-8]. On the other hand, very little has been done, concerning solvent effects in elimination reactions in mixed solvents. In this work we present the results of a

---

* In the presence of D_2O, unreacted p-nitrobenzyl chloride, recovered after partial conversion to p,p'-dinitrostilbene, was found to have incorporated deuterium as shown by infrared analysis.

5. Renfrow, W. B.,Jr. and Hauser, C. R.
J. Am. Chem. Soc., 59, 2308 (1937)
Bright, R. D. and Hauser, C. R.
ibid., 61, 618 (1939)

6. Tommila, E.
Acta Chem. Scand., 20, 923 (1966)
Tommila, E. and Pitkanen, I.
ibid., 20, 937 (1966)

7. Sadek, H., Halim, F., and Khalil, F.
Suomen Kemistilehti, B 36, 141 (1963)

8. Hyne, J. B., Golinkin, H. S., and Laidler, W. G.
J. Am. Chem. Soc., 88, 2104 (1966)

much-needed study, viz., a study of the influence of solvent composition on the p-nitrobenzyl chloride -- hydroxide ion reaction. The system dioxane-water was chosen since densities[9], and dielectric constant data are known[10], and since a study of the activity of hydroxide ion in such a system has been conducted previously[11].

---

9. Hans, S.
J. Chem. Eng. Data, 6, 19 (1961)

10. Akerlof, G. and Short, O. A.
J. Am. Chem. Soc., 58, 1241 (1936)

11. Nash, G. R. and Monk, C. B.
Trans. Faraday Soc., 54, 1657 (1958)

II. EXPERIMENTAL

Reagents. p-Nitrobenzyl chloride and dioxane were laboratory analytical reagent grades and were used without further purification. p-Nitrobenzyl chloride solutions were prepared by weighing exactly 3.4317 g of the reagent and dissolving in dioxane to get a 100 ml solution, 0.2000 M.

Silver nitrate solution for titration was prepared by weighing 0.8494 g of silver nitrate salt in water and making up the solution to 1000 ml. The salt had been previously dried at 120°C for 3 hours and cooled down to room temperature in a desiccator before weighing. The solution was standardized by electrometric titration against standard NaCl solution. The calculated normality of silver nitrate solution was 0.00505.

Sodium chloride solution for the standardization of the silver nitrate solution was prepared by dissolving 0.2923 g of NaCl (dried at 120°C for 2 hours and cooled at room temperature in a desiccator) in distilled water and diluting to one liter to get a 5.000×10^{-3} M standard solution.

Sodium hydroxide solution was prepared as follows:

(1) From a saturated NaOH solution* (set over night) the

---

* Solution was prepared by dissolving 50 g of NaOH in 50 ml freshly boiled and cooled distilled water.

clear supernatant liquid was siphoned (through glass wool) and the molarity estimated by acid-base titration with potassium hydrogen phthalate using phenolphthalein as indicator. The molarity was 0.5991 and was checked periodically and found to be constant.

(2) A certain volume of this NaOH was diluted to 2000 ml with CO_2-free, freshly-distilled water and the solution stored in a wax-coated-bottle.

(3) The wax-coated storage bottle, a 2-liter round-bottom-flask with a 24/40 standard taper, was made the reservoir for an automatic dispensing system which was operated exclusively under nitrogen atmosphere (Figure 1).

Sulfuric acid, used for quenching the reaction, was prepared by using the laboratory analytical reagent grade material, which was chloride-free. An approximately 1 M sulfuric acid solution was obtained by dissolving 56.4 ml of concentrated sulfuric acid in distilled water and diluting to one liter.

The buffer solution for the quinhydrone half-cell used in the electrometric titration of chloride ion was prepared by adding 6.5 ml of exactly one molar sulfuric acid and 10.21 g of potassium hydrogen phthalate to distilled water and diluting to one liter; the pH, measured on a Beckmann Model GS, was 3.42.

The electrometric determination of chloride ion was

Figure 1

AUTOMATIC BURETTE AND WAX-COATED BOTTLE FOR THE TRANSFER AND STORAGE OF STANDARD NaOH

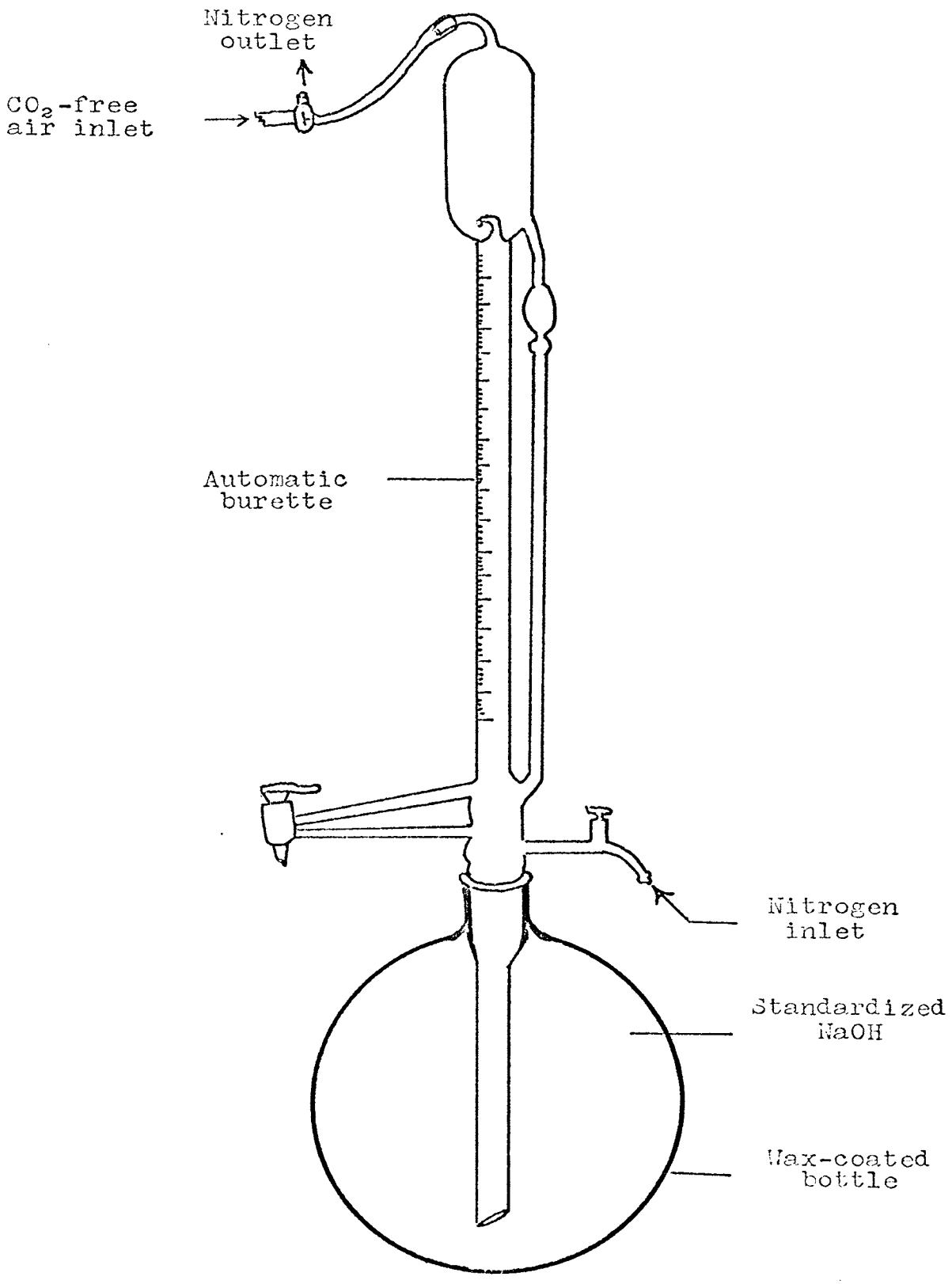

Nitrogen outlet
CO_2-free air inlet
Automatic burette
Nitrogen inlet
Standardized NaOH
Wax-coated bottle

Figure 1

described previously[12]. To our knowledge it is the fastest and one of the best methods for chloride determination. The apparatus used is shown in Figure 2.

Rate measurements. An X% (by volume) aqueous dioxane solution was made by mixing X ml of dioxane with (100 - X) ml water or NaOH in water solution. A mixture of (X - 5) ml dioxane, 16.70 ml 0.5991 N aqueous NaOH solution plus (83.30 - X) ml water was placed in a 100-ml round-bottom flask and allowed to reach thermal equilibrium in a well-stirred bath regulated at the desired temperature ±0.02°C. In a separate 150-ml long neck, round-bottom flask with a ground glass joint and glass stopper, 5 ml of the p-nitrobenzyl chloride solution in dioxane (1 mmole) were pipetted, and the solution was also thermostated for about 0.5 hour. To start a run, the bigger volume (NaOH in water-dioxane) was poured unto the smaller one ($ArCH_2Cl$ in dioxane), and the reaction mixture shaken vigorously to ensure good mixing. The solutions were always homogeneous at the beginning*. At suitable intervals of time, 5 ml portions were withdrawn, quenched in sulfuric acid solution

---

12. Chen, D. R.
The kinetics and mechanisms of the reaction of benzyl chloride with potassium t-butoxide in t-butyl alcohol Thesis (M.S.), University of Missouri at Rolla. 51 p. (With 4 figr., 2 tables) (1965)

* p,p'-Dinitrostilbene begins to precipitate in the reaction mixture after a few minutes but its presence as a precipitate does not interfere with the rate measurements.

Figure 2

ELECTROMETRIC METHOD FOR THE DETERMINATION OF CHLORIDE IONS

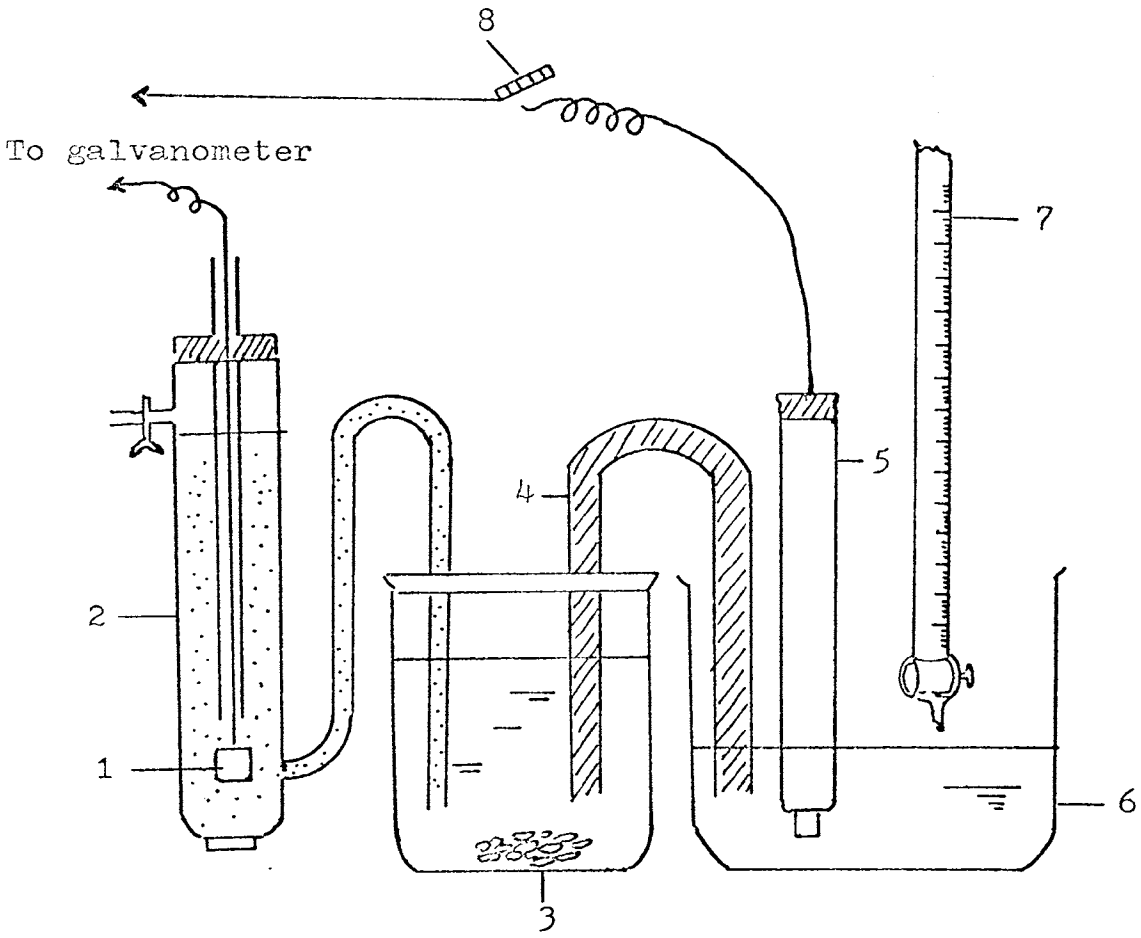


Fig. 2 ELECTROMETRIC METHOD FOR THE DETERMINATION OF CHLORIDE IONS

1. Platinum electrode
2. Quinhydrone half-cell
3. Saturated potassium nitrate solution
4. Agar-potassium nitrate bridge
5. Ag-AgCl electrode
6. Titration vessel
7. Burette
8. Key, single contact

(~1 M), and the liberated Cl^- titrated with Ag^+ using a Ag-AgCl electrode. The experimental results and the mathematical operations employed to calculate the second-order rate constants are described in Appendix I.

All experiments were run in duplicate, and some in triplicate. Twelve or thirteen samples were taken from the beginning till at least 70% reaction.

The initial concentrations of NaOH at the different temperatures were determined by titration of 50% solvent mixtures without added p-nitrobenzyl chloride.

III. RESULTS AND DISCUSSION

Table I contains a summary of the second-order rate constants and the corresponding activation parameters (Arrhenius activation energy, E_a, free energy of activation, ΔG^*, enthalpy of activation, ΔH^*, and entropy of activation, ΔS^*) for the eliminative condensation of p-nitrobenzyl chloride in aqueous dioxane solvent mixtures. The tabulated results represent the outcome of 25 experiments, run in duplicate or triplicate, each comprising a minimum of eleven samples. In other words, Table I is a condensate of approximately 500 experimental observations, each involving sampling, quenching and analysis for ionic chloride by electrometric titration.

The second-order-rate constants were calculated by use of the following equation:

$$- d[ArCH_2Cl]/dt = k[ArCH_2Cl][^-OH]$$

which, on integration, yields

$$k = \frac{1}{t(a - b)} \ln \frac{b(a - x)}{a(b - x)}$$

where a is the initial concentration of hydroxide ion,

b is the initial concentration of p-nitrobenzyl chloride

TABLE I SECOND-ORDER RATE CONSTANT AND ACTIVATION PARAMETERS FOR THE REACTION OF p-NITROBENZYL CHLORIDE WITH SODIUM HYDROXIDE IN AQUEOUS DIOXANE SOLVENT MIXTURES

Dioxane wt.%	°C	$k \pm \sigma k (10^3)$ $M^{-1} sec^{-1}$	$E_a \pm \sigma E_a$ Kcal $mole^{-1}$	$\Delta S^* \pm \sigma(\Delta S^*)$ cal $deg^{-1} mole^{-1}$	$H^* \pm \sigma(\Delta H^*)$ Kcal $mole^{-1}$	$\Delta G^* \pm \sigma(\Delta G^*)$ Kcal $mole^{-1}$
29.94	20	0.564±0.016	12.991±0.016	14.216±0.109	12.408±0.016	8.094±0.017
	25	0.724±0.026		14.436±0.124	12.398±0.016	8.094±0.021
	30	1.090±0.021		14.497±0.091	12.388±0.016	7.993±0.011
	35	1.540±0.050		14.456±0.117	12.378±0.016	7.924±0.019
	40	2.300±0.047		14.548±0.093	12.368±0.016	7.813±0.012
41.61	20	0.901±0.017	10.296±0.016	6.457±0.091	9.714±0.016	7.821±0.011
	25	1.190±0.044		6.387±0.127	9.704±0.016	7.800±0.022
	30	1.520±0.054		6.271±0.123	9.694±0.016	7.793±0.021
	35	2.080±0.045		6.310±0.097	9.684±0.016	7.740±0.013
	40	2.800±0.048		6.336±0.067	9.674±0.016	7.690±0.016
50.76	20	1.140±0.022	10.796±0.013	8.627±0.081	10.213±0.013	7.684±0.011
	25	1.300±0.028		8.257±0.067	10.203±0.013	7.747±0.013
	30	2.040±0.055		8.502±0.097	10.193±0.013	7.616±0.016
	35	2.770±0.040		8.499±0.071	10.183±0.013	7.564±0.006
	40	3.430±0.064		8.352±0.081	10.173±0.013	7.564±0.011
62.29	20	1.050±0.036	9.896±0.017	5.396±0.125	9.314±0.017	7.732±0.021
	25	1.270±0.025		5.174±0.097	9.304±0.017	7.761±0.012
	30	1.620±0.037		5.078±0.103	9.294±0.017	7.755±0.014
	35	2.430±0.050		5.321±0.099	9.284±0.017	7.644±0.013
	40	2.950±0.054		5.162±0.093	9.274±0.017	7.658±0.011
70.64	20	0.880±0.021	9.836±0.013	4.841±0.091	9.254±0.013	7.835±0.014
	25	1.050±0.021		4.596±0.083	9.244±0.013	7.874±0.012
	30	1.540±0.035		4.785±0.089	9.234±0.013	7.795±0.014
	35	1.930±0.036		4.669±0.081	9.224±0.013	7.795±0.013
	40	2.500±0.047		4.642±0.081	9.214±0.013	7.761±0.013

x is the concentration of already reacted material at time t

The Arrhenius activation energy, E_a, was calculated from the slope of the straight line obtained from a plot of lnk *vs.* 1/T in any one solvent medium. The enthalpy of activation, ΔH^*, was in turn calculated from E_a through use of the following equation:

$$\Delta H^* = E_a - RT$$

The free energy of activation, ΔG^*, and the entropy of activation, ΔS^*, were calculated by use of the Eyring equation,

$$k = \frac{RT}{Nh} e^{\Delta S^*/R} e^{-\Delta H^*/RT}$$

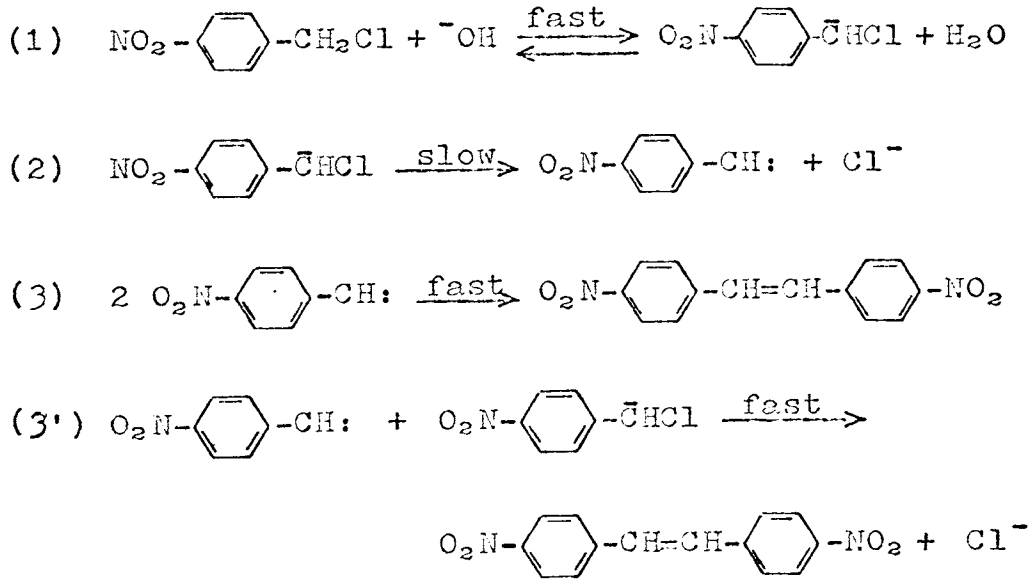
or $$\ln k = \ln \frac{RT}{Nh} + \frac{\Delta S^*}{R} - \frac{\Delta H^*}{RT}$$

in combination with the thermodynamical relationship,

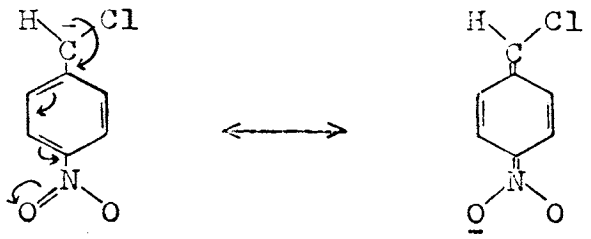
$$\Delta G^* = \Delta H^* - T\Delta S^*$$

Variations in the rate constants. An inspection of Table I reveals that the rate constants increase in the range from 30 to 50% dioxane and then decrease in the 60 and 70% dioxane at any one temperature. The change is more dramatic at 20° than at 40°C. For example, the rate constant in the 50% dioxane solvent mixture is approximately double that in

the 30% dioxane solvent mixture at 20°C, but the ratio is only about 1.5 at 40°C. The fact remains that the change in the rate constant does not simply parallel the variation in the percentage dioxane in the aqueous dioxane solvent mixture. As a matter of fact, there is no single property of the dioxane-water mixtures which changes in the same fashion as the rate constants of the studied reaction. However, an inspection of the steps of the mechanism of the studied transformation reveals that there are at least three factors which must be taken into consideration in any attempt to correlate rates with solvent composition.

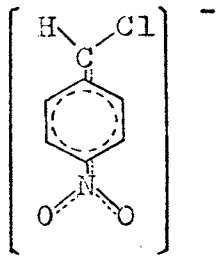


(a) First, the solvent effect on the rate-determining step, step (2) in the mechanism above. On the left hand side we have a species which is best represented by a resonance hybrid of the forms I and II



I II

A convenient way of representing the hybrid is shown in form III



III

where the negative charge is shown as dispersed over the entirety of the molecule. Such dispersal of charge requires little solvation[13]. On the other hand, the charged product on the right hand side of step (2) is a chloride ion, Cl^-, which demands a good deal of solvation by an appropriate solvent. In the mixed solvent system

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13. Ingold, C. K. "Structure and Mechanism in Organic Chemistry" Cornell University Press, Ithaca, N. Y., p. 324 (1953)

used in this study, dioxane is a very poor solvent for anions. Water, on the other hand, is an excellent solvent for anions[13]. So, here is a case of specific solute-solvent interaction in which the chloride ion will be heavily aquated or hydrated while the carbanion is only slightly so. It is readily seen that step (2) will be favored by an abundance of water in the solvent mixture. The failure to isolate the intermediate, R-C̄O-N-X, of the Hofmann reaction[5], except in non-aqueous media backs our argument.

(b) Second, step (1) in the presented mechanism is an equilibrium step as shown in earlier work[1]. The concentration of the carbanion, p-NO_2-C_6H_4-C̄HCl, will be inversely proportional to the concentration of water. Already we see that water in the reaction medium has opposite effects on steps (1) and (2); its abundance inhibits the formation of the important carbanion intermediate, yet it hastens its decomposition to products. The overall rate constant, which is a product of the equilibrium constant for step (1) and the rate constant for step (2) may be expected, therefore, to show little variation with solvent composition.

(c) Third, the activity or the effective concentration of hydroxide ion varies substantially with the change from 30 to 70% dioxane in the aqueous dioxane solvent mixture[11].

Nash and Monk reported that the dissociation constant of NaOH in 45% dioxane-water mixture at 25°C was 0.35 ± 0.05, but only 0.008 in a 70% dioxane-water mixture[11]. In this work, the initial concentrations of NaOH and p-nitrobenzyl chloride were approximately 0.1 and 0.01 M, respectively. In a 45% dioxane-water mixture, the effective concentration of hydroxide ion is calculated to be 0.082 M; this is about 80% of its stoichiometric concentration. However, in a 70% dioxane-water mixture, the effective concentration is calculated to be 0.0246 M, i.e., about 25% of the stoichiometric concentration of NaOH. Thus, a change from 30% to 70% dioxane in the reaction medium is apt to have a pronounced effect on the kinetics of the reaction in question.

In looking back on Table I, one may explain the increase in k in going from 30% to 50% dioxane by the predominance of factor (b), viz., enhancement of the concentration of the intermediate carbanion. The fact that the increase is relatively small may be accounted for by the partial compensation of factor (b) by factors (a) and (c), both of which would tend to decrease the rate constant. Above the 50% dioxane in the reaction mixture, the slight decrease may be accounted for by assuming that factor (b) is not adequate to compensate for the trends caused by (a) and (c).

The changes in k with the dielectric constant of the media are represented graphically in Figure 3. None of the available equations for the dependence of reaction rate constants on the dielectric constant can account for the observed point of inflexion around 50% dioxane. Such variation will, therefore, not be considered in this discussion.

Activation Parameters. There are two striking features in Table I regarding activation parameters. The free energy of activation, ΔG^*, is almost constant throughout the whole range of solvent mixtures and temperatures. An explanation of such constancy is not available at this time. The entropies of activation, ΔS^*, on the other hand, show a substantial decrease in going from 30% to 70% dioxane except for the 50% dioxane-water system. The change in the direction indicated may be accounted for by the greater orientation possible in the water-rich rather than in the dioxane-rich media. In summary, the variations in the rate-constants are mostly due to entropy changes in the system, which in turn are due to specific solute-solvent interactions.

Figure 3

VARIATION OF THE CALCULATED SECOND-ORDER RATE CONSTANTS WITH THE DIELECTRIC CONSTANT OF THE REACTION MEDIA

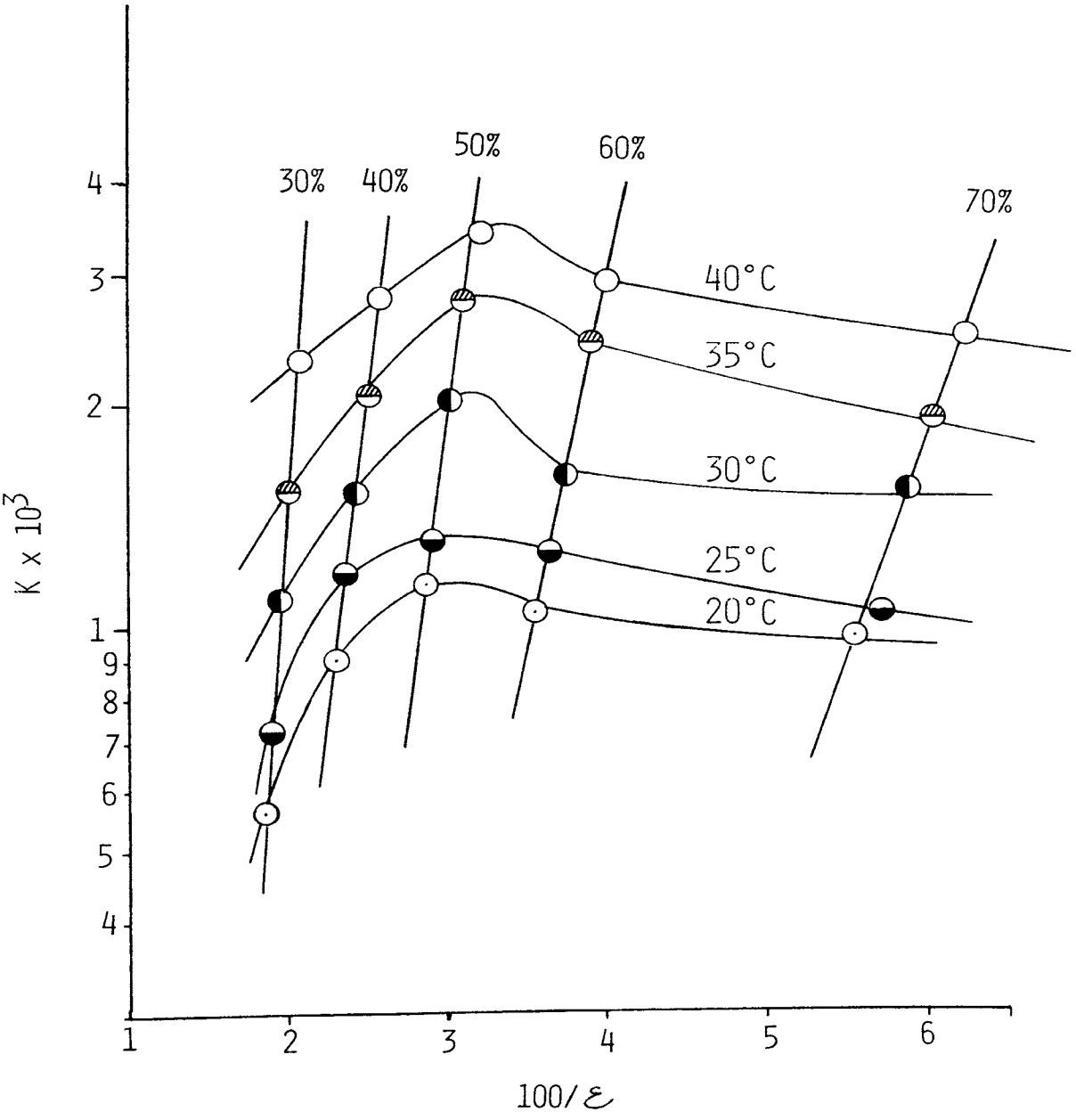
30%
40%
50%
60%
70%
40°C
35°C
30°C
25°C
20°C
K x 10³
4
3
2
1
9
8
7
6
5
4
1
2
3
4
5
6
100/ε

Figure 3

IV. APPENDICES

APPENDIX I DATA REDUCTION TECHNIQUES

I. A short review of linear least-squares regression[14].

The regression line of dependent variable (y) on independent variable (x) has the form of a linear, first-order model

$$y = \beta_o + \beta_1 x + \epsilon \qquad (I\text{-}1)$$

where β_o and β_1 are called the parameters of the model and ϵ is the increment by which any individual y may fall off the regression line. (A linear model is referred to linearity in the parameters. The value of the highest power of an independent variable x in the model is called the order of the model.)

The least-squares method is the way of fitting the best straight line to given data in order to relate the variables y and x. This method may be used to estimate the parameters which may be used to give a prediction of the true mean value of y by substitution of a value of x.

Having available n sets of observations (x_1, y_1), (x_2, y_2) ... (x_n, y_n), the equation may be written as

$$y_i = \beta_o + \beta_1 x_i + \epsilon_i \qquad (I\text{-}2)$$

---

14. Draper, N. R. and Smith, H. "Applied Regression Analysis" John Willey and Sons, Inc., New York, Chapters 1 and 2 (1966)

so that the sum of squares of deviations from the true line is

$$S = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \beta_o - \beta_1 x_i)^2 \qquad \text{(I-3)}$$

In order to get the least possible value of S, equation (I-3) may be differentiated first with respect to β_o and then to β_1 and set the results equal to zero. Now,

$$\frac{\partial S}{\partial \beta_o} = 0$$

$$\frac{\partial S}{\partial \beta_1} = 0 \qquad \text{(I-4)}$$

Through matrix formulation, it is very easy to solve equation (I-4) to find β_o and β_1 and give

$$\hat{\beta} = (X'X)^{-1}X'Y \qquad \text{(I-5)}$$

where

$$\hat{\beta} = \begin{bmatrix} \beta_o \\ \beta_1 \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

X' is the transpose of matrix X; $(X'X)^{-1}$ is the inverse of matrix $(X'X)$.

Equations (I-5) are called the normal equations which can be arranged in a computer programming for the computation of a parameters.

II. Standard deviation of β_i.

When we tackle the question of what measure of precision can be attached to our estimate of the regression line, we get to consider the relation of the sum of squares of deviations of the observations from the mean, $[\Sigma(y_i - \bar{y})^2]$, and the deviation of the observation from its predicted or fitted value, $[\Sigma(y_i - \hat{y}_i)^2]$, and the deviation of the predicted value of the observation from the mean, $[\Sigma(\hat{y}_i - \bar{y})^2]$. This relation may be expressed as

$$\begin{matrix}\text{Sum of squares} \\ \text{about the mean}\end{matrix} = \begin{matrix}\text{Sum of squares} \\ \text{about regression}\end{matrix} + \begin{matrix}\text{Sum of squares} \\ \text{due to regression}\end{matrix}$$

or

$$\Sigma(y_i - \bar{y})^2 = \Sigma(y_i - \hat{y}_i)^2 + \Sigma(\hat{y}_i - \bar{y})^2 \qquad \text{(II-1)}$$

This shows that, of the variation in y's about their mean, some of the variation can be ascribed to regression line

and some, to the fact that the actual observations do not all lie on the regression line, so that the fact of how small the quantity $(y_i - \hat{y}_i)^2$ may be observed is a measure of the precision of the regression line to the fitting of the data about this postulated model. Using equation (II-1) and considering the possible degrees of freedom, the variance due to regression from the variance about mean. employing alternative computational forms for the expressions of equation (II-1), the variance about regression may be written as

$$S^2 = \frac{[\Sigma x_i y_i - (\Sigma x_i)(\Sigma y_i)/n]^2}{\Sigma x_i^2 - (\Sigma x_i)^2/n} \qquad \text{(II-2)}$$

The estimated standard diviation of β_1 is given by

$$\text{est. s.d. } (\beta_1) = \frac{S}{[\Sigma(x_i - \bar{x})^2]^{\frac{1}{2}}} \qquad \text{(II-3)}$$

III. Confidence limits for [14,15].

Through the statistical theory it is possible to predict within what limits the observations is likely to agree with the regression line. Some fraction of risk, α, or percentage probility $(100 - 100\alpha)$ always involved in

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15. Fritz, J. S. and Schenk, G. H. "Quantitative Analytical Chemistry" Allyn and Bacon, Boston, p. 333-335 (1966)

such a prediction. The limits predicted for a certain risk or probability are called confidence limits. The limits depend on the t, or "Student's t" distribution curve which yields values for a constant called t. The t may be found by consulting table of percentage points of the t-distribution in most of statistics texts.

The way to assign $100(1 - \alpha)\%$ confidence limits for β_1 is to calculate

$$\beta_1 \pm \frac{tS}{\sqrt{n}}$$

where n is the number of measurements in sample; and t depends on α, and on the degrees of freedom (n - 2).

IV. Estimation of second-order rate constant, k, the standard diviation, and the confidence limits of k.

The rate constants were calculated by the second-order reaction rate equation,

$$k = \frac{1}{t(a - b)} \ln \frac{b(a - x)}{a(b - x)} .$$

This equation may be rearranged into the form,

$$\frac{1}{(a - b)} \ln \frac{b(a - x)}{a(b - x)} = kt . \qquad \text{(IV-1)}$$

The linear, first-order model can be applied to fit equation (IV-1) to give the form,

$$\frac{1}{(a - b)} \ln \frac{b(a - x)}{a(b - x)} = C + kt + \epsilon \qquad \text{(IV-2)}$$

where ϵ is the term of ramdom error, C and k are parameters; t and the formula at the left-hand side refer to x and y, respectively. The calculation of k and it's standard deviation with confidence limits may be arranged into a computational form in a computer programming based on the method mentioned in I to III exactly in this Appendix. The computer programming with the input data and output answers in the form of thesis-listing are also attached to this Appendix.

V. Estimation of the activation energy E_a and the calculation of ΔH^*, ΔS^*, and ΔG^*.

Using the Arrheneous equation,

$$\ln k = \ln A - \frac{E_a}{RT}$$

or $$\ln k = \ln A - \frac{E_a}{R}\left(\frac{1}{T}\right) \qquad \text{(V-1)}$$

In equation (V-1), E_a may also be observed as the parameter β_1 in the linear, first-order model and may be treated in the same way as the rate constant k in the last section.

The ΔH^*, ΔS^*, and ΔG^* may be obtained by the computations through the programming,

$$\Delta H^* = E_a - RT$$

$$\Delta S^* = R\ln\left(\frac{kh}{\not{k}T}\right) + \frac{\Delta H^*}{T}$$

$$\Delta G^* = \Delta H^* - T\Delta S^*$$

where $\not{k}$ is a Boltzmann constant, h is a Planck constant , and R is Gas constant.

The computer programming with the data input and the answer output in the form of thesis-listing are also attached to this Appendix.

```
C       CALCULATION OF SECOND ORDER RATE CONSTANTS
C       REACTION TYPE R(A)+S(B)=PRODUCTS
C       P-NITRO BENZYLCHLORIDE + NAOH = STILBENE  ( KEN K. HO )
        DIMENSION XML(300),H(300),X(300),Y(300),XSLOP(300),DEL(300),T(300)
        JJ=5
        TEMP=15.
        DO 8 NN=1,JJ
        TEMP=TEMP+5.
        READ (1,106)M
        READ (1,210) J
        DO 7 IQ=1,M
        WRITE (3,200) TEMP
        J=J+10
        WRITE (3,211) J
        WRITE (3,215)
        L=2
        SUMSL=0.
        SUMHL=0.
        DO 6 K=1,L
        READ (1,106) N
        READ (1,110) TS
        XN=N
        READ (1,100) (XML(I),I=1,N)
        READ (1,100) (H(I),I=1,N)
        READ (1,110) AX,B,CF
        A=AX*CF/5.
        WRITE (3,107) A,B
        DO 2 I=1,N
        T(I)=60.*H(I)
        X(I)=XML(I)*CF/5.
    2   Y(I)=ALOG(B*(A-X(I))/(A*(B-X(I))))/(A-B)
C       LEAST-SQUARES FITTING OF DATA
        SUMX=0.0
        SUMY=0.0
        SUMXY=0.0
        SUMX2=0.0
        SUMY2=0.0
        DO 3 I=1,N
        SUMX=T(I)+SUMX
        SUMY=Y(I)+SUMY
        SUMXY=T(I)*Y(I)+SUMXY
        SUMY2=Y(I)**2+SUMY2
    3   SUMX2=T(I)**2+SUMX2
        DEM=XN*SUMX2-SUMX**2
        SLOPE=(XN*SUMXY-SUMX*SUMY)/DEM
        CONST=(SUMX2*SUMY-SUMX*SUMXY)/DEM
        WRITE (3,101) SLOPE,CONST
        SUMSL=SUMSL+SLOPE
        HL=(ALOG(B/(2.*B-A)))/(SLOPE*(A-B))
        WRITE (3,240)HL
        SUMHL=SUMHL+HL
C       CALCULATE OF INDIVIDUAL SLOPES
        DO 4 I=1,N
        CALCK=Y(I)/T(I)
```

```
      DEL(I)=SLOPE-CALCK
    4 WRITE (3,102) T(I), CALCK,DEL(I)
C     STATISTICAL TREATMENT OF THE DATA
      DEL1=0.0
      DEL2=0.0
      DO 5 I=1,N
      DSLOP=ABS(DEL(I))
    5 DEL1=DSLOP+DEL1
      ADEV=DEL1/XN
      WRITE (3,103) ADEV
      A=SUMY2-(SUMY**2)/XN
      B1=SUMXY
      B2=SUMX*SUMY/XN
      B3=SUMX2
      B4=(SUMX**2)/XN
      B=((B1-B2)**2)/(B3-B4)
      S2=(A-B)/(XN-2)
      STD=SQRT(S2/(B3-B4))
      WRITE (3,104)STD
      ST=TS*STD/SQRT(XN)
      WRITE (3,105) ST
    6 WRITE (3,215)
      AVHL=SUMHL/L
      WRITE (3,250)AVHL
      ASLOPE=SUMSL/L
    7 WRITE (3,230) ASLOPE
    8 WRITE (3,215)
      RETURN
  100 FORMAT(6F10.2)
  101 FORMAT(2X,7HSLOPE =,E13.5,14HLITER/MOLE-SEC,5X,9HCONSTANT=,E13.5)
  102 FORMAT(2X,5HTIME=,F10.3,2X,10HEXP CONST=,E11.5,2X,4HDEV=,E12.5)
  103 FORMAT(2X,19HAVERAGE DEVIATION =,E13.5)
  104 FORMAT(2X,20HSTANDARD DEVIATION =,E13.5)
  105 FORMAT(2X,38HAT 95% CONFIDENCE LIMIT K=SLOPE+(OR -),E14.8)
  106 FORMAT(I6)
  107 FORMAT(1X,13HCONC OF PCL =,F8.5,5X14HCONC OF NAOH =,F8.5)
  110 FORMAT(6F12.6)
  200 FORMAT(15H1TEMPERATURE IS,F6.1,1X,1HC)
  210 FORMAT(I8)
  211 FORMAT(1X,19HDIOXANE-AQ SYSTEM %,I3)
  215 FORMAT('/')
  230 FORMAT(1X,9HAVESLOPE=,E13.3)
  240 FORMAT(2X,10HHALF LIFE=,E13.3)
  250 FORMAT(1X,18HAVERAGE HALF LIFE=,E13.3)
      END
     5
      20
     13
       2.179
      0.47       1.26       1.84       2.34       2.85       3.45
      3.89       4.28       4.75       5.17       5.45       5.98
      6.55
     13.27      29.90      45.00      60.83      79.42     105.13
    129.50     154.80     180.87     218.88     249.30     289.92
```

```
342.22
    9.74        0.0952    0.5086E-2
13
   2.179
  0.55        1.30        1.93        2.32        2.95        3.43
  3.99        4.36        4.81        5.23        5.55        6.13
  6.49
 13.73       29.92       44.22       61.22       79.25      105.23
129.98      155.05      184.33      219.33      252.65      281.30
342.27
    9.76        0.0952    0.5086E-2
13
   2.179
  0.96        1.86        2.61        3.30        3.78        4.29
  4.59        4.98        5.57        6.19        6.70        7.13
  7.60
 16.11       30.63       45.05       61.37       75.02       89.95
106.53      121.02      150.22      180.60      212.70      249.13
282.00
    9.81        0.0952    0.5086E-2
13
   2.179
  1.01        1.92        2.62        3.22        3.75        4.17
  4.57        4.93        5.60        6.05        6.52        6.9
  7.40
 16.57       31.37       45.22       61.77       75.83       89.97
106.57      122.17      152.33      181.25      213.92      249.15
281.52
    9.77        0.0952    0.5086E-2
12
   2.201
  1.29        2.42        3.18        3.83        4.28        5.11
  5.57        6.17        6.55        6.86        7.10        7.65
 16.28       31.75       45.90       59.42       77.15      100.05
121.03      143.28      162.80      184.47      203.95      219.92
    9.87        0.0952    0.5086E-2
12
   2.201
  1.37        2.48        3.19        3.74        4.21        5.01
  5.49        6.03        6.54        6.88        7.20        7.55
 16.90       32.40       46.30       60.32       77.72      101.53
121.65      143.98      163.40      185.75      203.63      219.53
    9.82        0.0952    0.5086E-2
12
   2.201
  1.44        2.64        3.44        3.98        4.43        4.79
  5.29        5.58        5.85        6.13        6.87        7.02
 14.60       30.05       46.40       59.03       74.08       89.65
104.63      119.73      134.72      149.42      173.65      192.82
   10.10        0.0952    0.5041E-2
12
   2.201
  1.53        1.65        3.43        3.94        4.33        4.74
  5.22        5.57        5.76        6.33        6.83        7.03
```

```
 15.72      30.78      46.47      59.33      74.40      90.52
104.32     120.52     134.95     149.68     175.08     199.50
   10.12       0.0952    0.5041E-2
12
   2.201
  1.30       2.37       3.06       3.61       4.21       4.72
  5.13       5.66       5.94       6.43       6.90       7.38
 11.75      24.65      39.18      55.40      75.10      99.53
126.15     147.55     164.49     192.28     217.78     244.22
   10.04       0.0952    0.5086E-2
12
   2.201
  1.43       2.33       3.01       3.51       4.02       4.69
  5.21       5.61       6.06       6.52       6.96       7.42
 12.52      24.08      39.88      55.17      74.95      99.17
125.27     146.10     166.67     190.77     216.65     243.60
   10.04       0.0952    0.5086E-2
 5
  20
13
   2.179
  0.76       2.10       2.87       3.24       4.02       4.21
  4.85       5.14       5.59       5.86       6.23       6.52
  7.17
 11.95      29.80      47.18      63.48      79.27      95.77
120.22     138.87     165.78     191.22     222.27     251.05
306.70
    9.68       0.0981    0.5086E-2
12
   2.201
  0.84       2.10       2.77       3.46       4.29       4.71
  5.08       5.51       6.00       6.28       6.60       7.21
 11.52      29.58      47.53      63.35      96.62     120.70
137.60     166.11     192.10     223.50     250.82     311.35
    9.70       0.0981    0.5086E-2
12
   2.201
  1.19       2.57       3.44       4.16       4.64       5.25
  5.74       6.21       6.49       6.83       7.00       7.23
 10.78      22.78      36.63      49.98      63.13      86.55
104.33     117.32     137.07     152.11     167.47     190.35
    9.86       0.0981    0.5086E-2
12
   2.201
  1.21       2.34       3.42       4.16       4.55       5.39
  5.85       6.18       6.48       6.82       7.10       7.45
 10.80      22.22      36.93      51.02      64.07      86.58
104.22     117.45     132.43     153.28     167.45     190.53
    9.85       0.0981    0.5086E-2
12
   2.201
  1.31       2.41       3.73       4.43       5.19       5.91
  6.54       6.80       7.22       7.30       7.51       7.69
 11.67      23.57      44.73      59.13      78.10     100.90
```

```
124.53     141.43     160.33     165.67     175.65     185.75
    9.98        0.0981    0.5051E-2
11
   2.228
  1.48       2.70       3.79       4.72       5.92       6.55
  6.85       6.98       7.30       7.48       7.67
 12.30      24.38      45.33      59.20     100.27     125.75
141.35     151.37     165.05     175.03     185.73
   10.00        0.0981    0.5051E-2
12
   2.201
  2.39       3.23       4.10       4.95       5.50       5.82
  6.27       6.62       7.01       7.49       7.65       7.94
 17.18      28.05      44.65      61.83      82.43     100.82
120.33     135.11     148.03     171.45     182.13     200.10
    9.91        0.0981    0.5086E-2
12
   2.201
  2.55       3.25       4.11       4.58       5.34       5.95
  6.26       6.64       6.98       7.50       7.60       7.85
 17.37      27.17      44.48      62.00      82.25     101.18
119.93     135.57     147.02     170.55     181.60     199.83
    9.86        0.0981    0.5086E-2
12
   2.201
  1.77       2.62       3.09       3.57       4.12       4.76
  5.22       6.17       6.50       7.02       7.39       7.60
 11.58      27.58      36.11      52.17      70.03      87.87
112.70     138.13     159.62     181.10     201.68     214.60
    9.91        0.0981    0.5086E-2
12
   2.201
  1.52       2.49       3.06       3.42       4.00       4.60
  5.20       5.78       6.28       6.84       7.13       7.36
 12.10      27.07      35.90      52.08      69.62      87.72
112.22     137.75     158.35     186.83     201.68     214.70
    9.96        0.0981    0.5086E-2
 5
  20
12
   2.201
  1.67       2.58       3.50       4.03       4.59       4.92
  5.27       5.88       6.24       6.63       7.13       7.36
 14.90      25.48      41.65      56.33      71.92      84.83
101.48     123.13     144.82     166.52     195.73     211.08
    9.68        0.0984    0.5051E-2
12
   2.201
  1.85       2.56       3.51       4.01       4.57       4.90
  5.35       5.85       6.41       6.76       7.18       7.41
 15.20      25.55      41.67      56.88      71.82      85.93
101.72     122.57     145.33     166.78     197.11     210.92
    9.66        0.0984    0.5051E-2
12
```

```
   2.201
  1.69        3.31        4.16        4.75        5.01        5.44
  5.94        6.02        6.42        6.60        6.82        7.31
  9.98       24.72       36.68       47.27       55.45       64.69
 80.33       87.48       94.87      106.67      118.72      130.46
    9.92         0.0984    0.5051E-2
12
   2.201
  1.72        3.22        4.11        4.56        4.93        5.34
  5.62        6.08        6.26        6.65        6.86        7.24
 10.22       23.70       36.22       46.90       54.48       64.53
 74.38       87.05       94.30      106.52      118.20      130.59
    9.89         0.0984    0.5051E-2
12
   2.201
  2.09        3.46        4.51        5.00        5.26        5.83
  6.00        6.35        6.84        7.09        7.21        7.36
  8.70       18.03       29.73       36.93       42.05       52.07
 61.20       70.00       80.80       87.08       93.58      104.27
   10.00         0.0984    0.5051E-2
12
   2.201
  2.73        3.82        4.60        5.06        5.45        5.93
  6.16        6.44        6.88        7.10        7.29        7.54
 12.38       20.85       32.32       39.50       46.27       57.19
 64.85       73.58       83.35       90.10       96.03      103.44
    9.99         0.0984    0.5051E-2
11
   2.228
  2.33        3.53        4.32        5.60        6.07        6.63
  6.86        7.13        7.27        7.68        7.95
 10.58       24.42       36.42       75.02       84.87       95.83
104.63      115.27      123.92      136.45      146.92
   10.06         0.0984    0.5051E-2
11
   2.228
  2.28        3.71        4.33        5.76        6.07        6.65
  6.77        7.07        7.33        7.67        7.87
 10.73       24.11       36.62       70.78       84.08       95.19
103.65      113.80      122.38      135.93      143.17
   10.08         0.0984    0.5051E-2
12
   2.201
  2.29        3.30        3.62        4.37        5.20        5.56
  5.81        6.14        6.47        6.68        6.96        7.39
  9.97       20.22       33.62       46.77       61.05       71.28
 80.56       89.85      101.10      110.77      118.25      130.65
    9.98         0.0984    0.5051E-2
12
   2.201
  2.29        3.30        3.62        4.37        5.20        5.56
  5.81        6.14        6.47        6.68        6.96        7.39
  9.97       20.22       33.62       46.77       61.05       71.28
 80.56       89.85      101.10      110.77      118.25      130.65
```

```
    9.98        0.0984    0.5051E-2
 5
  20
12
   2.201
  1.90        3.16        3.68        4.15        4.58        5.14
  5.46        5.80        6.26        6.56        7.14        7.42
 10.73       22.85       30.67       39.10       49.02       58.65
 69.18       78.43       94.97      108.28      129.82      143.30
    9.70        0.0990    0.5051E-2
12
   2.201
  1.83        3.65        3.14        4.17        4.68        5.07
  5.45        5.75        6.23        6.68        7.06        7.47
 10.78       22.13       30.05       38.30       48.45       58.13
 68.27       78.77       95.13      107.11      130.08      148.40
    9.72        0.0990    0.5051E-2
12
   2.201
  2.12        3.24        4.12        4.58        5.02        5.47
  5.79        6.21        6.64        7.06        7.38        7.41
  9.08       17.02       26.30       32.73       41.33       49.69
 55.88       65.90       77.53       89.68       99.62      118.59
    9.95        0.0990    0.5051E-2
12
   2.201
  1.95        3.08        3.94        4.92        5.31        5.75
  6.18        6.61        6.80        7.05        7.31        7.62
  9.37       16.10       25.57       40.05       47.57       54.97
 64.98       76.42       83.62       88.80       98.38      108.20
   10.01        0.0990    0.5051E-2
12
   2.201
  1.73        2.94        3.52        4.13        4.66        5.12
  5.47        5.90        6.51        7.03        7.45        7.74
  5.73       11.77       16.65       23.13       29.11       35.15
 40.88       46.78       56.78       67.37       76.17       86.43
   10.05        0.0990    0.5051E-2
12
   2.201
  1.80        2.97        3.62        4.17        4.62        5.14
  5.50        5.95        6.50        6.99        7.42        7.74
  5.92       11.83       16.72       23.25       29.18       35.23
 41.02       46.88       56.85       67.55       76.22       86.25
   10.04        0.0990    0.5051E-2
12
   2.201
  2.08        3.27        3.74        4.17        4.52        5.03
  5.54        6.12        6.69        7.02        7.40        7.66
  5.80       11.78       16.45       21.27       26.72       32.90
 40.27       50.17       62.45       73.55       83.02       89.50
   10.04        0.0990    0.5051E-2
12
   2.201
```

```
  1.99        3.00        3.52        3.95        4.40        4.84
  5.26        5.94        6.62        7.05        7.32        7.47
  5.95       11.83       16.33       20.58       26.67       33.08
 40.58       50.03       62.78       74.20       83.15       88.83
   10.02         0.0990      0.5051E-2
12
   2.201
  1.46        2.11        2.64        3.11        3.59        4.42
  5.08        5.65        6.06        6.67        7.19        7.53
  5.48       11.55       18.65       26.32       33.55       40.48
 59.77       72.25       82.55       99.02      113.53      124.80
    9.88         0.0990      0.5041E-2
12
   2.201
  1.61        2.25        2.80        3.20        3.54        4.44
  5.26        5.84        6.29        6.91        7.40        7.83
  5.62       11.90       19.08       26.13       34.03       40.62
 59.83       72.30       83.75       99.88      113.75      125.00
    9.91         0.0990      0.5051E-2
 5
  20
12
   2.201
  2.05        3.18        4.02        4.61        5.09        5.56
  5.96        6.22        6.58        6.95        7.22        7.45
  7.73       15.53       24.27       31.82       39.85       48.32
 56.28       65.53       72.02       81.15       91.50       98.23
    9.79         0.0988      0.5041E-2
12
   2.201
  2.15        3.26        4.09        4.70        5.16        5.61
  6.00        6.28        6.74        7.08        7.35        7.53
  8.11       15.88       24.77       32.18       40.45       48.60
 56.82       64.75       72.58       82.23       91.77       98.80
    9.80         0.0988      0.5041E-2
12
   2.201
  1.75        2.88        3.52        4.16        4.65        5.09
  5.50        5.78        6.58        7.06        7.39        7.70
  5.80       11.50       16.67       23.20       29.10       35.10
 40.91       46.69       56.81       67.42       76.10       86.38
    9.98         0.0988      0.5051E-2
12
   2.201
  1.80        2.96        3.68        4.17        4.59        5.17
  5.49        5.93        6.48        6.95        7.39        7.80
  5.90       11.81       16.80       23.30       29.15       35.23
 41.01       46.85       56.80       67.50       76.17       86.30
    9.99         0.0988      0.5051E-2
12
   2.201
  2.10        3.12        3.94        4.72        5.05        5.58
  5.93        6.26        6.69        7.29        7.60        7.81
  5.65       10.18       16.08       23.32       27.00       31.95
```

```
 37.17      42.22      48.18      57.45      66.22      72.36
   10.02       0.0988    0.5041E-2
12
   2.201
  1.76       2.79       3.64       4.30       4.96       5.15
  5.64       5.96       6.40       6.96       7.47       7.83
  4.93       9.78      15.57      21.78      26.77      30.93
 36.07      40.70      47.22      56.38      66.07      72.43
    9.93       0.0988    0.5041E-2
12
   2.201
  1.68       2.51       3.19       3.78       4.34       5.03
  5.30       5.83       6.46       6.84       7.32       7.79
  4.73       9.15      14.38      19.63      24.45      29.68
 38.57      46.13      54.72      63.03      71.90      81.43
   10.01       0.0988    0.5051E-2
12
   2.201
  1.74       2.61       3.25       3.87       4.30       4.74
  5.37       5.93       6.40       6.93       7.36       7.83
  5.07       9.78      14.50      19.17      24.72      30.07
 37.63      46.30      54.15      62.63      72.07      81.35
   10.01       0.0988    0.5051E-2
12
   2.201
  2.10       3.24       3.75       4.20       4.56       5.06
  5.62       6.15       6.68       7.18       7.54       7.63
  5.82      11.75      16.47      21.30      28.75      32.88
 40.30      50.15      62.45      73.62      83.10      89.33
   10.00       0.0988    0.5051E-2
12
   2.201
  2.15       3.05       3.55       4.01       4.42       4.82
  5.25       6.00       6.63       7.12       7.38       7.54
  6.10      11.87      16.35      20.62      26.68      33.05
 40.55      50.10      62.78      74.25      83.18      89.88
   10.02       0.0988    0.5051E-2
```

```
TEMPERATURE IS  20.0 C
DIOXANE-AQ SYSTEM % 30

CONC OF HCL = 0.00991      CONC OF NAOH = 0.09520
 SLOPE =  0.56745E-03LITER/MOLE-SEC      CONSTANT=  0.73406E 00
 HALF LIFE=     0.132E 05
 TIME=    796.200   EXP CONST=0.65415E-03   DEV=-0.86696E-04
 TIME=   1793.999   EXP CONST=0.81676E-03   DEV=-0.24931E-03
 TIME=   2700.000   EXP CONST=0.82298E-03   DEV=-0.25552E-03
 TIME=   3649.800   EXP CONST=0.80129E-03   DEV=-0.23383E-03
 TIME=   4765.199   EXP CONST=0.77563E-03   DEV=-0.20818E-03
 TIME=   6307.796   EXP CONST=0.74296E-03   DEV=-0.17551E-03
 TIME=   7770.000   EXP CONST=0.70519E-03   DEV=-0.13774E-03
 TIME=   9288.000   EXP CONST=0.67153E-03   DEV=-0.10407E-03
 TIME=  10852.190   EXP CONST=0.66628E-03   DEV=-0.98828E-04
 TIME=  13132.790   EXP CONST=0.62484E-03   DEV=-0.57386E-04
 TIME=  14958.000   EXP CONST=0.59567E-03   DEV=-0.28214E-04
 TIME=  17395.190   EXP CONST=0.59703E-03   DEV=-0.29571E-04
 TIME=  20533.190   EXP CONST=0.59593E-03   DEV=-0.28473E-04
 AVERAGE DEVIATION =  0.13026E-03
 STANDARD DEVIATION =  0.15164E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.91640890E-05

CONC OF HCL = 0.00993      CONC OF NAOH = 0.09520
 SLOPE =  0.56063E-03LITER/MOLE-SEC      CONSTANT=  0.83706E 00
 HALF LIFE=     0.134E 05
 TIME=    823.800   EXP CONST=0.74179E-03   DEV=-0.18115E-03
 TIME=   1795.199   EXP CONST=0.84240E-03   DEV=-0.28177E-03
 TIME=   2653.199   EXP CONST=0.88176E-03   DEV=-0.32113E-03
 TIME=   3673.199   EXP CONST=0.79641E-03   DEV=-0.22578E-03
 TIME=   4755.000   EXP CONST=0.77539E-03   DEV=-0.21476E-03
 TIME=   6316.796   EXP CONST=0.75066E-03   DEV=-0.19035E-03
 TIME=   7798.796   EXP CONST=0.72487E-03   DEV=-0.16424E-03
 TIME=   9303.000   EXP CONST=0.68599E-03   DEV=-0.12536E-03
 TIME=  11059.790   EXP CONST=0.66398E-03   DEV=-0.10329E-03
 TIME=  13159.790   EXP CONST=0.63277E-03   DEV=-0.72134E-04
 TIME=  15158.990   EXP CONST=0.60318E-03   DEV=-0.42551E-04
 TIME=  17478.000   EXP CONST=0.59899E-03   DEV=-0.38356E-04
 TIME=  20536.190   EXP CONST=0.58340E-03   DEV=-0.22772E-04
 AVERAGE DEVIATION =  0.15259E-03
 STANDARD DEVIATION =  0.16097E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.97282220E-05

 AVERAGE HALF LIFE=     0.133E 05
 AVESLOPE=     0.564E-03
```

```
TEMPERATURE IS  20.0 C
DIOXANE-AQ SYSTEM % 40

CONC OF RCL = 0.00998      CONC OF NAOH = 0.09520
 SLOPE =  0.92945E-03LITER/MOLE-SEC      CONSTANT=  0.76193E 00
 HALF LIFE=     0.807E 04
 TIME=    966.600   EXP CONST=0.11250E-02   DEV=-0.19558E-03
 TIME=   1837.800   EXP CONST=0.12141E-02   DEV=-0.28463E-03
 TIME=   2703.000   EXP CONST=0.12200E-02   DEV=-0.29058E-03
 TIME=   3682.199   EXP CONST=0.11924E-02   DEV=-0.26292E-03
 TIME=   4501.199   EXP CONST=0.11612E-02   DEV=-0.23174E-03
 TIME=   5391.000   EXP CONST=0.11347E-02   DEV=-0.20529E-03
 TIME=   6391.796   EXP CONST=0.10659E-02   DEV=-0.13646E-03
 TIME=   7261.199   EXP CONST=0.10567E-02   DEV=-0.12722E-03
 TIME=   9013.199   EXP CONST=0.10122E-02   DEV=-0.82743E-04
 TIME=  10836.000   EXP CONST=0.10055E-02   DEV=-0.76014E-04
 TIME=  12761.990   EXP CONST=0.98796E-03   DEV=-0.58513E-04
 TIME=  14941.790   EXP CONST=0.95680E-03   DEV=-0.27349E-04
 TIME=  16920.000   EXP CONST=0.97488E-03   DEV=-0.45429E-04
 AVERAGE DEVIATION =   0.15573E-03
 STANDARD DEVIATION =   0.15198E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.91850450E-05

CONC OF RCL = 0.00994      CONC OF NAOH = 0.09520
 SLOPE =  0.87165E-03LITER/MOLE-SEC      CONSTANT=  0.96550E 00
 HALF LIFE=     0.861E 04
 TIME=    994.200   EXP CONST=0.11593E-02   DEV=-0.28764E-03
 TIME=   1882.199   EXP CONST=0.12343E-02   DEV=-0.36261E-03
 TIME=   2713.199   EXP CONST=0.12268E-02   DEV=-0.35520E-03
 TIME=   3706.200   EXP CONST=0.11546E-02   DEV=-0.28292E-03
 TIME=   4549.796   EXP CONST=0.11426E-02   DEV=-0.27119E-03
 TIME=   5393.199   EXP CONST=0.11102E-02   DEV=-0.23852E-03
 TIME=   6394.199   EXP CONST=0.10650E-02   DEV=-0.19331E-03
 TIME=   7330.199   EXP CONST=0.10373E-02   DEV=-0.16563E-03
 TIME=   9139.796   EXP CONST=0.10154E-02   DEV=-0.14172E-03
 TIME=  10875.000   EXP CONST=0.96931E-03   DEV=-0.97657E-04
 TIME=  12835.190   EXP CONST=0.93978E-03   DEV=-0.68129E-04
 TIME=  14943.000   EXP CONST=0.90138E-03   DEV=-0.29728E-04
 TIME=  16801.199   EXP CONST=0.92651E-03   DEV=-0.54664E-04
 AVERAGE DEVIATION =   0.19607E-03
 STANDARD DEVIATION =   0.19166E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.11582720E-04

 AVERAGE HALF LIFE=     0.834E 04
 AVESLOPE=     0.901E-03
```

TEMPERATURE IS 20.0 C
DIOXANE-AQ SYSTEM % 50

CONC OF HCL = 0.01004 CONC OF NAOH = 0.09520
SLOPE = 0.11333E-02LITER/MOLE-SEC CONSTANT= 0.86025E 00
HALF LIFE= 0.662E 04

TIME=	976.800	EXP CONST=0.15169E-02	DEV=-0.38367E-03
TIME=	1905.000	EXP CONST=0.15724E-02	DEV=-0.43911E-03
TIME=	2753.999	EXP CONST=0.15107E-02	DEV=-0.37747E-03
TIME=	3565.199	EXP CONST=0.14799E-02	DEV=-0.34661E-03
TIME=	4628.996	EXP CONST=0.13234E-02	DEV=-0.19017E-03
TIME=	6003.000	EXP CONST=0.13167E-02	DEV=-0.18339E-03
TIME=	7261.796	EXP CONST=0.12443E-02	DEV=-0.11107E-03
TIME=	8596.796	EXP CONST=0.12470E-02	DEV=-0.11377E-03
TIME=	9768.000	EXP CONST=0.12226E-02	DEV=-0.89279E-04
TIME=	11068.190	EXP CONST=0.11792E-02	DEV=-0.45875E-04
TIME=	12236.990	EXP CONST=0.11436E-02	DEV=-0.10326E-04
TIME=	13195.190	EXP CONST=0.12519E-02	DEV=-0.11858E-03

AVERAGE DEVIATION = 0.20078E-03
STANDARD DEVIATION = 0.29337E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.18640080E-04

CONC OF HCL = 0.00999 CONC OF NAOH = 0.09520
SLOPE = 0.11417E-02LITER/MOLE-SEC CONSTANT= 0.75643E 00
HALF LIFE= 0.657E 04

TIME=	1013.999	EXP CONST=0.15683E-02	DEV=-0.42659E-03
TIME=	1943.999	EXP CONST=0.15951E-02	DEV=-0.45337E-03
TIME=	2778.000	EXP CONST=0.15120E-02	DEV=-0.37123E-03
TIME=	3619.200	EXP CONST=0.14223E-02	DEV=-0.28060E-03
TIME=	4663.199	EXP CONST=0.12932E-02	DEV=-0.15144E-03
TIME=	6091.796	EXP CONST=0.12690E-02	DEV=-0.12725E-03
TIME=	7298.996	EXP CONST=0.12194E-02	DEV=-0.77670E-04
TIME=	8638.796	EXP CONST=0.12029E-02	DEV=-0.61153E-04
TIME=	9803.996	EXP CONST=0.12259E-02	DEV=-0.84195E-04
TIME=	11145.000	EXP CONST=0.11895E-02	DEV=-0.47802E-04
TIME=	12217.790	EXP CONST=0.11922E-02	DEV=-0.50491E-04
TIME=	13170.000	EXP CONST=0.12302E-02	DEV=-0.88453E-04

AVERAGE DEVIATION = 0.18502E-03
STANDARD DEVIATION = 0.17699E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.11245710E-04

AVERAGE HALF LIFE= 0.660E 04
AVESLOPE= 0.114E-02

```
TEMPERATURE IS   20.0 C
DIOXANE-AQ SYSTEM % 60

CONC OF RCL = 0.01018      CONC OF NAOH = 0.09520
 SLOPE =  0.10304E-02LITER/MOLE-SEC      CONSTANT=  0.13650E 01
 HALF LIFE=     0.729E 04
 TIME=    876.000   EXP CONST=0.18590E-02   DEV=-0.82864E-03
 TIME=   1803.000   EXP CONST=0.17916E-02   DEV=-0.76117E-03
 TIME=   2783.999   EXP CONST=0.16026E-02   DEV=-0.57215E-03
 TIME=   3541.799   EXP CONST=0.15207E-02   DEV=-0.49031E-03
 TIME=   4444.796   EXP CONST=0.14007E-02   DEV=-0.37027E-03
 TIME=   5378.996   EXP CONST=0.12921E-02   DEV=-0.26169E-03
 TIME=   6277.796   EXP CONST=0.12819E-02   DEV=-0.25151E-03
 TIME=   7183.796   EXP CONST=0.12167E-02   DEV=-0.18632E-03
 TIME=   8083.199   EXP CONST=0.11665E-02   DEV=-0.13614E-03
 TIME=   8965.199   EXP CONST=0.11370E-02   DEV=-0.10664E-03
 TIME=  10418.990   EXP CONST=0.12018E-02   DEV=-0.17136E-03
 TIME=  11569.190   EXP CONST=0.11289E-02   DEV=-0.98484E-04
 AVERAGE DEVIATION =   0.35289E-03
 STANDARD DEVIATION =   0.30470E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.19359590E-04

CONC OF RCL = 0.01020      CONC OF NAOH = 0.09520
 SLOPE =  0.10738E-02LITER/MOLE-SEC      CONSTANT=  0.91944E 00
 HALF LIFE=     0.699E 04
 TIME=    943.200   EXP CONST=0.18408E-02   DEV=-0.76708E-03
 TIME=   1846.799   EXP CONST=0.10215E-02   DEV= 0.52218E-04
 TIME=   2708.199   EXP CONST=0.15904E-02   DEV=-0.51660E-03
 TIME=   3550.800   EXP CONST=0.14891E-02   DEV=-0.41538E-03
 TIME=   4463.996   EXP CONST=0.13479E-02   DEV=-0.27417E-03
 TIME=   5431.199   EXP CONST=0.12571E-02   DEV=-0.18334E-03
 TIME=   6259.199   EXP CONST=0.12564E-02   DEV=-0.18261E-03
 TIME=   7231.199   EXP CONST=0.12017E-02   DEV=-0.12791E-03
 TIME=   8096.596   EXP CONST=0.11321E-02   DEV=-0.58286E-04
 TIME=   8980.796   EXP CONST=0.11957E-02   DEV=-0.12109E-03
 TIME=  10504.790   EXP CONST=0.11743E-02   DEV=-0.10058E-03
 TIME=  11614.790   EXP CONST=0.11233E-02   DEV=-0.49564E-04
 AVERAGE DEVIATION =   0.23748E-03
 STANDARD DEVIATION =   0.41107E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.26116170E-04

 AVERAGE HALF LIFE=     0.714E 04
 AVESLOPE=     0.105E-02
```

```
TEMPERATURE IS   20.0 C
DIOXANE-AQ SYSTEM % 70

CONC OF HCL = 0.01021      CONC OF NAOH = 0.09520
 SLOPE =   0.86583E-03LITER/MOLE-SEC      CONSTANT=  0.15225E 01
 HALF LIFE=     0.867E 04
 TIME=    705.000   EXP CONST=0.20809E-02   DEV=-0.12151E-02
 TIME=   1478.999   EXP CONST=0.19381E-02   DEV=-0.10723E-02
 TIME=   2350.799   EXP CONST=0.16532E-02   DEV=-0.78735E-03
 TIME=   3323.999   EXP CONST=0.14381E-02   DEV=-0.57229E-03
 TIME=   4506.000   EXP CONST=0.12992E-02   DEV=-0.43338E-03
 TIME=   5971.796   EXP CONST=0.11494E-02   DEV=-0.28358E-03
 TIME=   7568.996   EXP CONST=0.10243E-02   DEV=-0.15852E-03
 TIME=   8853.000   EXP CONST=0.10196E-02   DEV=-0.15378E-03
 TIME=   9869.398   EXP CONST=0.98956E-03   DEV=-0.12373E-03
 TIME=  11536.790   EXP CONST=0.97064E-03   DEV=-0.10481E-03
 TIME=  13066.790   EXP CONST=0.97772E-03   DEV=-0.11189E-03
 TIME=  14653.190   EXP CONST=0.10006E-02   DEV=-0.13480E-03
 AVERAGE DEVIATION =   0.42929E-03
 STANDARD DEVIATION =   0.24482E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.15555C0E-04

CONC OF HCL = 0.01021      CONC OF NAOH = 0.09520
 SLOPE =   0.89492E-03LITER/MOLE-SEC      CONSTANT=  0.13761E 01
 HALF LIFE=     0.839E 04
 TIME=    751.200   EXP CONST=0.21656E-02   DEV=-0.12707E-02
 TIME=   1444.800   EXP CONST=0.19452E-02   DEV=-0.10503E-02
 TIME=   2392.800   EXP CONST=0.15918E-02   DEV=-0.69666E-03
 TIME=   3310.199   EXP CONST=0.13932E-02   DEV=-0.49829E-03
 TIME=   4496.996   EXP CONST=0.12234E-02   DEV=-0.32853E-03
 TIME=   5950.199   EXP CONST=0.11431E-02   DEV=-0.24821E-03
 TIME=   7516.199   EXP CONST=0.10558E-02   DEV=-0.16092E-03
 TIME=   8766.000   EXP CONST=0.10153E-02   DEV=-0.12038E-03
 TIME=  10000.190   EXP CONST=0.10100E-02   DEV=-0.11504E-03
 TIME=  11446.190   EXP CONST=0.10032E-02   DEV=-0.10829E-03
 TIME=  12998.990   EXP CONST=0.99966E-03   DEV=-0.10474E-03
 TIME=  14616.000   EXP CONST=0.10150E-02   DEV=-0.12007E-03
 AVERAGE DEVIATION =   0.40185E-03
 STANDARD DEVIATION =   0.17410E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.11061950E-04

AVERAGE HALF LIFE=     0.853E 04
AVESLOPE=     0.880E-03
```

```
TEMPERATURE IS  25.0 C
DIOXANE-AQ SYSTEM % 30

CONC OF RCL = 0.00985      CONC OF NAOH = 0.09810
 SLOPE =  0.72010E-03LITER/MOLE-SEC      CONSTANT=  0.15177E 01
 HALF LIFE=     0.101E 05
 TIME=    717.000   EXP CONST=0.11671E-02   DEV=-0.44705E-03
 TIME=   1788.000   EXP CONST=0.14102E-02   DEV=-0.69015E-03
 TIME=   2830.799   EXP CONST=0.12867E-02   DEV=-0.56662E-03
 TIME=   3808.799   EXP CONST=0.11107E-02   DEV=-0.39063E-03
 TIME=   4756.199   EXP CONST=0.11770E-02   DEV=-0.45694E-03
 TIME=   5746.199   EXP CONST=0.10375E-02   DEV=-0.31742E-03
 TIME=   7213.199   EXP CONST=0.10110E-02   DEV=-0.29094E-03
 TIME=   8232.199   EXP CONST=0.95515E-03   DEV=-0.23505E-03
 TIME=   9946.796   EXP CONST=0.91339E-03   DEV=-0.19329E-03
 TIME=  11473.190   EXP CONST=0.85638E-03   DEV=-0.13628E-03
 TIME=  13336.190   EXP CONST=0.81983E-03   DEV=-0.99729E-04
 TIME=  15063.000   EXP CONST=0.78947E-03   DEV=-0.69372E-04
 TIME=  18401.990   EXP CONST=0.78355E-03   DEV=-0.63458E-04
 AVERAGE DEVIATION =  0.30438E-03
 STANDARD DEVIATION =  0.28301E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.17103720E-04

CONC OF RCL = 0.00987      CONC OF NAOH = 0.09810
 SLOPE =  0.72738E-03LITER/MOLE-SEC      CONSTANT=  0.14230E 01
 HALF LIFE=     0.100E 05
 TIME=    691.200   EXP CONST=0.13418E-02   DEV=-0.61440E-03
 TIME=   1774.800   EXP CONST=0.14174E-02   DEV=-0.69004E-03
 TIME=   2851.799   EXP CONST=0.12206E-02   DEV=-0.49319E-03
 TIME=   3801.000   EXP CONST=0.12064E-02   DEV=-0.47906E-03
 TIME=   5797.199   EXP CONST=0.10525E-02   DEV=-0.32515E-03
 TIME=   7241.996   EXP CONST=0.96187E-03   DEV=-0.23449E-03
 TIME=   8256.000   EXP CONST=0.94394E-03   DEV=-0.21656E-03
 TIME=   9966.597   EXP CONST=0.88766E-03   DEV=-0.16028E-03
 TIME=  11526.000   EXP CONST=0.88454E-03   DEV=-0.15716E-03
 TIME=  13410.000   EXP CONST=0.82416E-03   DEV=-0.96780E-04
 TIME=  15049.190   EXP CONST=0.80570E-03   DEV=-0.78317E-04
 TIME=  18691.000   EXP CONST=0.77786E-03   DEV=-0.50485E-04
 AVERAGE DEVIATION =  0.29965E-03
 STANDARD DEVIATION =  0.24506E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.15570440E-04

AVERAGE HALF LIFE=     0.100E 05
AVESLOPE=     0.724E-03
```

```
TEMPERATURE IS  25.0 C
DIOXANE-AQ SYSTEM % 40

CONC OF HCL = 0.01003      CONC OF NAOH = 0.09810
 SLOPE =  0.11596E-02LITER/MOLE-SEC      CONSTANT=  0.17571E 01
 HALF LIFE=      0.627E 04
 TIME=    646.800   EXP CONST=0.20399E-02   DEV=-0.88026E-03
 TIME=   1366.799   EXP CONST=0.22843E-02   DEV=-0.11247E-02
 TIME=   2197.800   EXP CONST=0.20291E-02   DEV=-0.86941E-03
 TIME=   2998.799   EXP CONST=0.19080E-02   DEV=-0.74840E-03
 TIME=   3787.800   EXP CONST=0.17587E-02   DEV=-0.59903E-03
 TIME=   5193.000   EXP CONST=0.15399E-02   DEV=-0.38028E-03
 TIME=   6259.796   EXP CONST=0.14715E-02   DEV=-0.31190E-03
 TIME=   7039.199   EXP CONST=0.14956E-02   DEV=-0.33597E-03
 TIME=   8224.199   EXP CONST=0.13960E-02   DEV=-0.22638E-03
 TIME=   9126.597   EXP CONST=0.13766E-02   DEV=-0.21693E-03
 TIME=  10048.190   EXP CONST=0.13134E-02   DEV=-0.15378E-03
 TIME=  11421.000   EXP CONST=0.12363E-02   DEV=-0.76695E-04
 AVERAGE DEVIATION =  0.49364E-03
 STANDARD DEVIATION =  0.48752E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.30975520E-04

CONC OF HCL = 0.01002      CONC OF NAOH = 0.09810
 SLOPE =  0.12298E-02LITER/MOLE-SEC      CONSTANT=  0.14914E 01
 HALF LIFE=      0.592E 04
 TIME=    648.000   EXP CONST=0.20752E-02   DEV=-0.84541E-03
 TIME=   1333.199   EXP CONST=0.21006E-02   DEV=-0.97085E-03
 TIME=   2215.799   EXP CONST=0.20003E-02   DEV=-0.77051E-03
 TIME=   3061.200   EXP CONST=0.18717E-02   DEV=-0.64193E-03
 TIME=   3944.200   EXP CONST=0.16876E-02   DEV=-0.45738E-03
 TIME=   5104.796   EXP CONST=0.16059E-02   DEV=-0.37617E-03
 TIME=   6253.199   EXP CONST=0.15224E-02   DEV=-0.29279E-03
 TIME=   7046.996   EXP CONST=0.14839E-02   DEV=-0.25413E-03
 TIME=   7945.796   EXP CONST=0.14331E-02   DEV=-0.20336E-03
 TIME=   9196.796   EXP CONST=0.13648E-02   DEV=-0.13503E-03
 TIME=  10046.996   EXP CONST=0.13553E-02   DEV=-0.12557E-03
 TIME=  11481.799   EXP CONST=0.13225E-02   DEV=-0.92692E-04
 AVERAGE DEVIATION =  0.42219E-03
 STANDARD DEVIATION =  0.39729E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.24607550E-04

 AVERAGE HALF LIFE=     0.609E 04
 AVESLOPE=    0.119E-02
```

```
TEMPERATURE IS   25.0 C
DIOXANE-AQ SYSTEM % 50

CONC OF RCL = 0.01009      CONC OF NAOH = 0.09810
 SLOPE =  0.13193E-02LITER/MOLE-SEC      CONSTANT=  0.11278E 01
 HALF LIFE=     0.551E 04
 TIME=    700.200   EXP CONST=0.20628E-02   DEV=-0.74355E-03
 TIME=   1414.200   EXP CONST=0.20185E-02   DEV=-0.69927E-03
 TIME=   2683.799   EXP CONST=0.18154E-02   DEV=-0.49610E-03
 TIME=   3547.800   EXP CONST=0.17296E-02   DEV=-0.41029E-03
 TIME=   4686.000   EXP CONST=0.16466E-02   DEV=-0.32727E-03
 TIME=   6053.996   EXP CONST=0.15219E-02   DEV=-0.20264E-03
 TIME=   7471.796   EXP CONST=0.15135E-02   DEV=-0.19427E-03
 TIME=   8485.796   EXP CONST=0.14341E-02   DEV=-0.11478E-03
 TIME=   9619.796   EXP CONST=0.14268E-02   DEV=-0.10752E-03
 TIME=   9940.199   EXP CONST=0.14134E-02   DEV=-0.94130E-04
 TIME=  10538.990   EXP CONST=0.14185E-02   DEV=-0.99266E-04
 TIME=  11145.000   EXP CONST=0.14122E-02   DEV=-0.92889E-04
 AVERAGE DEVIATION =   0.29850E-03
 STANDARD DEVIATION =   0.24470E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.15547480E-04

CONC OF RCL = 0.01010      CONC OF NAOH = 0.09810
 SLOPE =  0.12816E-02LITER/MOLE-SEC      CONSTANT=  0.14149E 01
 HALF LIFE=     0.568E 04
 TIME=    738.000   EXP CONST=0.22298E-02   DEV=-0.94823E-03
 TIME=   1462.800   EXP CONST=0.22259E-02   DEV=-0.94420E-03
 TIME=   2719.800   EXP CONST=0.18243E-02   DEV=-0.54267E-03
 TIME=   3551.999   EXP CONST=0.18838E-02   DEV=-0.60225E-03
 TIME=   6016.199   EXP CONST=0.15746E-02   DEV=-0.29295E-03
 TIME=   7545.000   EXP CONST=0.14977E-02   DEV=-0.21608E-03
 TIME=   8481.000   EXP CONST=0.14498E-02   DEV=-0.16824E-03
 TIME=   9082.199   EXP CONST=0.14048E-02   DEV=-0.12320E-03
 TIME=   9903.000   EXP CONST=0.14128E-02   DEV=-0.13121E-03
 TIME=  10501.790   EXP CONST=0.14047E-02   DEV=-0.12314E-03
 TIME=  11142.790   EXP CONST=0.14016E-02   DEV=-0.11999E-03
 AVERAGE DEVIATION =   0.38292E-03
 STANDARD DEVIATION =   0.32187E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.21622020E-04

AVERAGE HALF LIFE=     0.560E 04
AVESLOPE=     0.130E-02
```

```
TEMPERATURE IS  25.0 C
DIOXANE-AQ SYSTEM % 60

CONC OF HCL = 0.01008      CONC OF NAOH = 0.09810
 SLOPE =  0.12650E-02LITER/MOLE-SEC      CONSTANT=  0.19468E 01
 HALF LIFE=      0.575E 04
 TIME=   1030.799   EXP CONST=0.27652E-02   DEV=-0.15002E-02
 TIME=   1683.000   EXP CONST=0.24326E-02   DEV=-0.11676E-02
 TIME=   2678.999   EXP CONST=0.20202E-02   DEV=-0.81522E-03
 TIME=   3709.800   EXP CONST=0.19583E-02   DEV=-0.69331E-03
 TIME=   4945.796   EXP CONST=0.17250E-02   DEV=-0.46005E-03
 TIME=   6049.199   EXP CONST=0.15452E-02   DEV=-0.28026E-03
 TIME=   7219.796   EXP CONST=0.14703E-02   DEV=-0.20530E-03
 TIME=   8106.597   EXP CONST=0.14457E-02   DEV=-0.18070E-03
 TIME=   8881.796   EXP CONST=0.14753E-02   DEV=-0.21035E-03
 TIME=  10296.990   EXP CONST=0.14677E-02   DEV=-0.20271E-03
 TIME=  10927.790   EXP CONST=0.14509E-02   DEV=-0.18589E-03
 TIME=  12006.000   EXP CONST=0.14474E-02   DEV=-0.18246E-03
 AVERAGE DEVIATION =  0.50700E-03
 STANDARD DEVIATION =  0.29536E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.18766350E-04

CONC OF HCL = 0.01003      CONC OF NAOH = 0.09810
 SLOPE =  0.12668E-02LITER/MOLE-SEC      CONSTANT=  0.19441E 01
 HALF LIFE=      0.574E 04
 TIME=   1042.199   EXP CONST=0.29682E-02   DEV=-0.17014E-02
 TIME=   1630.199   EXP CONST=0.25466E-02   DEV=-0.12798E-02
 TIME=   2668.799   EXP CONST=0.21091E-02   DEV=-0.84231E-03
 TIME=   3720.000   EXP CONST=0.17578E-02   DEV=-0.49101E-03
 TIME=   4935.000   EXP CONST=0.16635E-02   DEV=-0.39670E-03
 TIME=   6070.796   EXP CONST=0.16109E-02   DEV=-0.34406E-03
 TIME=   7195.796   EXP CONST=0.14840E-02   DEV=-0.21714E-03
 TIME=   8134.199   EXP CONST=0.14626E-02   DEV=-0.19576E-03
 TIME=   8821.199   EXP CONST=0.14874E-02   DEV=-0.22061E-03
 TIME=  10233.000   EXP CONST=0.14967E-02   DEV=-0.22988E-03
 TIME=  10896.000   EXP CONST=0.14496E-02   DEV=-0.18276E-03
 TIME=  11989.790   EXP CONST=0.14257E-02   DEV=-0.15887E-03
 AVERAGE DEVIATION =  0.52169E-03
 STANDARD DEVIATION =  0.20232E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.12855190E-04

 AVERAGE HALF LIFE=      0.575E 04
 AVESLOPE=     0.127E-02
```

```
TEMPERATURE IS  25.0 C
DIOXANE-AQ SYSTEM % 70

CONC OF HCL = 0.01008      CONC OF NAOH = 0.09810
 SLOPE =  0.10956E-02LITER/MOLE-SEC      CONSTANT=  0.11753E 01
 HALF LIFE=     0.664E 04
 TIME=    694.800   EXP CONST=0.20144E-02   DEV=-0.18189E-02
 TIME=   1654.800   EXP CONST=0.19189E-02   DEV=-0.82330E-03
 TIME=   2166.599   EXP CONST=0.17887E-02   DEV=-0.69314E-03
 TIME=   3130.199   EXP CONST=0.14843E-02   DEV=-0.38867E-03
 TIME=   4201.796   EXP CONST=0.13350E-02   DEV=-0.23944E-03
 TIME=   5272.199   EXP CONST=0.13014E-02   DEV=-0.20581E-03
 TIME=   6761.996   EXP CONST=0.11634E-02   DEV=-0.67834E-04
 TIME=   8287.796   EXP CONST=0.12452E-02   DEV=-0.14957E-03
 TIME=   9577.199   EXP CONST=0.11828E-02   DEV=-0.87166E-04
 TIME=  10866.000   EXP CONST=0.12094E-02   DEV=-0.11381E-03
 TIME=  12100.796   EXP CONST=0.12107E-02   DEV=-0.11513E-03
 TIME=  12876.000   EXP CONST=0.12125E-02   DEV=-0.11693E-03
 AVERAGE DEVIATION =   0.49163E-03
 STANDARD DEVIATION =   0.22270E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.14149510E-04

CONC OF HCL = 0.01013      CONC OF NAOH = 0.09810
 SLOPE =  0.99879E-03LITER/MOLE-SEC      CONSTANT=  0.12223E 01
 HALF LIFE=     0.729E 04
 TIME=    726.000   EXP CONST=0.23441E-02   DEV=-0.13453E-02
 TIME=   1624.200   EXP CONST=0.18304E-02   DEV=-0.83161E-03
 TIME=   2153.999   EXP CONST=0.17670E-02   DEV=-0.76818E-03
 TIME=   3124.800   EXP CONST=0.13988E-02   DEV=-0.40011E-03
 TIME=   4177.199   EXP CONST=0.12822E-02   DEV=-0.28367E-03
 TIME=   5263.199   EXP CONST=0.12227E-02   DEV=-0.22402E-03
 TIME=   6733.199   EXP CONST=0.11529E-02   DEV=-0.15416E-03
 TIME=   8265.000   EXP CONST=0.11082E-02   DEV=-0.11042E-03
 TIME=   9501.000   EXP CONST=0.11107E-02   DEV=-0.11194E-03
 TIME=  11210.796   EXP CONST=0.11025E-02   DEV=-0.10371E-03
 TIME=  12100.796   EXP CONST=0.11089E-02   DEV=-0.11113E-03
 TIME=  12851.999   EXP CONST=0.11151E-02   DEV=-0.11735E-03
 AVERAGE DEVIATION =   0.31685E-03
 STANDARD DEVIATION =   0.14631E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.10185790E-04

 AVERAGE HALF LIFE=     0.696E 04
 AVESLOPE=     0.105E-02
```

```
TEMPERATURE IS   30.0 C
DIOXANE-AQ SYSTEM 4-30

CONC OF HCL = 0.00976      CONC OF NAOH = 0.00840
 SLOPE =   0.10735E-02LITER/MOLE-SEC      CONSTANT=  0.17058E 01
 HALF LIFE=      0.675E 04
 TIME=    894.000   EXP CONST=0.21720E-02   DEV=-0.10984E-02
 TIME=   1528.799   EXP CONST=0.20987E-02   DEV=-0.10162E-02
 TIME=   2408.999   EXP CONST=0.18410E-02   DEV=-0.78751E-03
 TIME=   3379.800   EXP CONST=0.16565E-02   DEV=-0.59297E-03
 TIME=   4315.199   EXP CONST=0.15546E-02   DEV=-0.48111E-03
 TIME=   5029.796   EXP CONST=0.14587E-02   DEV=-0.38522E-03
 TIME=   6088.796   EXP CONST=0.13529E-02   DEV=-0.28040E-03
 TIME=   7387.796   EXP CONST=0.12331E-02   DEV=-0.16058E-03
 TIME=   8649.199   EXP CONST=0.12576E-02   DEV=-0.18495E-03
 TIME=   9991.199   EXP CONST=0.12247E-02   DEV=-0.15123E-03
 TIME=  11743.799   EXP CONST=0.12087E-02   DEV=-0.13518E-03
 TIME=  12664.799   EXP CONST=0.12027E-02   DEV=-0.12923E-03
 AVERAGE DEVIATION =   0.45759E-03
 STANDARD DEVIATION =   0.24199E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.15375290E-04

CONC OF HCL = 0.00976      CONC OF NAOH = 0.00840
 SLOPE =   0.11062E-02LITER/MOLE-SEC      CONSTANT=  0.16560E 01
 HALF LIFE=      0.655E 04
 TIME=    912.000   EXP CONST=0.23925E-02   DEV=-0.12833E-02
 TIME=   1533.600   EXP CONST=0.21468E-02   DEV=-0.96367E-03
 TIME=   2502.199   EXP CONST=0.19719E-02   DEV=-0.78668E-03
 TIME=   3412.800   EXP CONST=0.18200E-02   DEV=-0.63278E-03
 TIME=   4359.199   EXP CONST=0.16913E-02   DEV=-0.50541E-03
 TIME=   5155.796   EXP CONST=0.16035E-02   DEV=-0.42251E-03
 TIME=   6103.199   EXP CONST=0.15174E-02   DEV=-0.34121E-03
 TIME=   7264.199   EXP CONST=0.14229E-02   DEV=-0.25211E-03
 TIME=   8710.796   EXP CONST=0.13218E-02   DEV=-0.16111E-03
 TIME=  10078.796   EXP CONST=0.12496E-02   DEV=-0.10026E-03
 TIME=  11423.996   EXP CONST=0.11934E-02   DEV=-0.05184E-03
 TIME=  12466.196   EXP CONST=0.11884E-02   DEV=-0.05221E-03
 AVERAGE DEVIATION =   0.41417E-03
 STANDARD DEVIATION =   0.18485E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.11463742E-04

 AVERAGE HALF LIFE=      0.665E 04
 AVESLOPE=     0.1099E-02
```

TEMPERATURE IS 30.0 C
DIOXANE-AQ SYSTEM % 40

CONC OF HCL = 0.01002 CONC OF NAOH = 0.09840
SLOPE = 0.15138E-02LITER/MOLE-SEC CONSTANT= 0.20167E 01
HALF LIFE= 0.479E 04
TIME= 508.800 EXP CONST=0.31775E-02 DEV=-0.16637E-02
TIME= 1483.199 EXP CONST=0.28333E-02 DEV=-0.13195E-02
TIME= 2206.799 EXP CONST=0.25765E-02 DEV=-0.10567E-02
TIME= 2836.200 EXP CONST=0.24084E-02 DEV=-0.88662E-03
TIME= 3326.999 EXP CONST=0.22122E-02 DEV=-0.69843E-03
TIME= 4000.799 EXP CONST=0.20857E-02 DEV=-0.57187E-03
TIME= 4819.799 EXP CONST=0.19963E-02 DEV=-0.48249E-03
TIME= 5248.796 EXP CONST=0.18750E-02 DEV=-0.36121E-03
TIME= 5692.199 EXP CONST=0.19353E-02 DEV=-0.42154E-03
TIME= 6400.199 EXP CONST=0.18111E-02 DEV=-0.29729E-03
TIME= 7123.199 EXP CONST=0.17323E-02 DEV=-0.21853E-03
TIME= 8376.000 EXP CONST=0.17186E-02 DEV=-0.20478E-03
AVERAGE DEVIATION = 0.62188E-03
STANDARD DEVIATION = 0.58917E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.37434130E-04

CONC OF HCL = 0.00999 CONC OF NAOH = 0.09840
SLOPE = 0.15233E-02LITER/MOLE-SEC CONSTANT= 0.19314E 01
HALF LIFE= 0.474E 04
TIME= 613.200 EXP CONST=0.31956E-02 DEV=-0.16722E-02
TIME= 1421.999 EXP CONST=0.28658E-02 DEV=-0.13425E-02
TIME= 2173.199 EXP CONST=0.25712E-02 DEV=-0.10479E-02
TIME= 2813.999 EXP CONST=0.23921E-02 DEV=-0.85876E-03
TIME= 3268.799 EXP CONST=0.22693E-02 DEV=-0.73598E-03
TIME= 3990.000 EXP CONST=0.20769E-02 DEV=-0.54360E-03
TIME= 4462.796 EXP CONST=0.19781E-02 DEV=-0.45483E-03
TIME= 5223.000 EXP CONST=0.19263E-02 DEV=-0.40288E-03
TIME= 5658.000 EXP CONST=0.18770E-02 DEV=-0.34759E-03
TIME= 6391.199 EXP CONST=0.18460E-02 DEV=-0.32259E-03
TIME= 7091.996 EXP CONST=0.17726E-02 DEV=-0.24901E-03
TIME= 8314.799 EXP CONST=0.16985E-02 DEV=-0.17315E-03
AVERAGE DEVIATION = 0.69786E-03
STANDARD DEVIATION = 0.45556E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.31486720E-04

AVERAGE HALF LIFE= 0.476E 04
AVESLOPE= 0.152E-02

```
TEMPERATURE IS   30.0 C
DIOXANE-AQ SYSTEM % 50

CONC OF HCL = 0.01010        CONC OF NAOH = 0.09840
 SLOPE =  0.20525E-02LITER/MOLE-SEC      CONSTANT=  0.22194E 01
 HALF LIFE=     0.353E 04
 TIME=    522.000    EXP CONST=0.46162E-02   DEV=-0.25637E-02
 TIME=   1081.799    EXP CONST=0.40670E-02   DEV=-0.20145E-02
 TIME=   1783.799    EXP CONST=0.35062E-02   DEV=-0.14538E-02
 TIME=   2215.799    EXP CONST=0.32734E-02   DEV=-0.12210E-02
 TIME=   2576.999    EXP CONST=0.30849E-02   DEV=-0.98447E-03
 TIME=   3038.199    EXP CONST=0.28432E-02   DEV=-0.74075E-03
 TIME=   3671.999    EXP CONST=0.26300E-02   DEV=-0.52751E-03
 TIME=   4200.000    EXP CONST=0.25359E-02   DEV=-0.48345E-03
 TIME=   4848.000    EXP CONST=0.25211E-02   DEV=-0.46864E-03
 TIME=   5224.796    EXP CONST=0.25119E-02   DEV=-0.45948E-03
 TIME=   5614.796    EXP CONST=0.24197E-02   DEV=-0.36727E-03
 TIME=   6022.199    EXP CONST=0.23568E-02   DEV=-0.30437E-03
 AVERAGE DEVIATION =   0.97408E-03
 STANDARD DEVIATION =   0.66954E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.42540730E-04

CONC OF HCL = 0.01009        CONC OF NAOH = 0.09840
 SLOPE =  0.20211E-02LITER/MOLE-SEC      CONSTANT=  0.23448E 01
 HALF LIFE=     0.359E 04
 TIME=    742.800    EXP CONST=0.44329E-02   DEV=-0.24118E-02
 TIME=   1251.000    EXP CONST=0.39990E-02   DEV=-0.19789E-02
 TIME=   1939.200    EXP CONST=0.33207E-02   DEV=-0.12996E-02
 TIME=   2370.000    EXP CONST=0.31196E-02   DEV=-0.10985E-02
 TIME=   2776.200    EXP CONST=0.29820E-02   DEV=-0.96092E-03
 TIME=   3430.799    EXP CONST=0.27569E-02   DEV=-0.73575E-03
 TIME=   3801.000    EXP CONST=0.26000E-02   DEV=-0.57893E-03
 TIME=   4414.796    EXP CONST=0.24794E-02   DEV=-0.45772E-03
 TIME=   5001.000    EXP CONST=0.24765E-02   DEV=-0.45543E-03
 TIME=   5406.000    EXP CONST=0.24394E-02   DEV=-0.41842E-03
 TIME=   5761.796    EXP CONST=0.24185E-02   DEV=-0.39734E-03
 TIME=   6208.796    EXP CONST=0.24165E-02   DEV=-0.39537E-03
 AVERAGE DEVIATION =   0.93234E-03
 STANDARD DEVIATION =   0.43998E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.27948800E-04

AVERAGE HALF LIFE=     0.356E 04
AVESLOPE=     0.204E-02
```

TEMPERATURE IS 30.0 C
DIOXANE-AQ SYSTEM # 60

CONC OF HCL = 0.01016 CONC OF NAOH = 0.09840
SLOPE = 0.16186E-02LITER/MOLE-SEC CONSTANT= 0.18649E 01
HALF LIFE= 0.448E 04
TIME= 634.800 EXP CONST=0.42713E-02 DEV=-0.26527E-02
TIME= 1465.199 EXP CONST=0.30572E-02 DEV=-0.14385E-02
TIME= 2195.199 EXP CONST=0.26748E-02 DEV=-0.10562E-02
TIME= 4501.199 EXP CONST=0.18989E-02 DEV=-0.28032E-03
TIME= 5092.199 EXP CONST=0.19150E-02 DEV=-0.29634E-03
TIME= 5748.000 EXP CONST=0.19660E-02 DEV=-0.34739E-03
TIME= 6277.796 EXP CONST=0.19359E-02 DEV=-0.31732E-03
TIME= 6916.199 EXP CONST=0.18968E-02 DEV=-0.27817E-03
TIME= 7435.199 EXP CONST=0.18366E-02 DEV=-0.21803E-03
TIME= 8186.996 EXP CONST=0.18817E-02 DEV=-0.26309E-03
TIME= 8815.199 EXP CONST=0.18404E-02 DEV=-0.22182E-03
AVERAGE DEVIATION = 0.66998E-03
STANDARD DEVIATION = 0.37638E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.25284150E-04

CONC OF HCL = 0.01019 CONC OF NAOH = 0.09840
SLOPE = 0.16218E-02LITER/MOLE-SEC CONSTANT= 0.19834E 01
HALF LIFE= 0.447E 04
TIME= 643.800 EXP CONST=0.40882E-02 DEV=-0.24762E-02
TIME= 1446.599 EXP CONST=0.32921E-02 DEV=-0.16703E-02
TIME= 2197.199 EXP CONST=0.26615E-02 DEV=-0.10397E-02
TIME= 4246.796 EXP CONST=0.20989E-02 DEV=-0.47713E-03
TIME= 5044.796 EXP CONST=0.19266E-02 DEV=-0.30483E-03
TIME= 5710.796 EXP CONST=0.19004E-02 DEV=-0.27751E-03
TIME= 6218.996 EXP CONST=0.18985E-02 DEV=-0.27672E-03
TIME= 6829.000 EXP CONST=0.18814E-02 DEV=-0.25961E-03
TIME= 7342.796 EXP CONST=0.18845E-02 DEV=-0.26273E-03
TIME= 8155.796 EXP CONST=0.18748E-02 DEV=-0.25304E-03
TIME= 8590.199 EXP CONST=0.18914E-02 DEV=-0.26961E-03
AVERAGE DEVIATION = 0.69705E-03
STANDARD DEVIATION = 0.36783E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.24676000E-04

AVERAGE HALF LIFE= 0.448E 04
AVESLOPE= 0.162E-02

TEMPERATURE IS 30.0 C
DIOXANE-AQ SYSTEM V/V 70

CONC OF RCL = 0.01008 CONC OF NAOH = 0.09840
SLOPE = 0.15385E-02LITER/MOLE-SEC CONSTANT= 0.18509E 01
HALF LIFE= 0.471E 04
TIME= 598.200 EXP CONST=0.44835E-02 DEV=-0.29453E-02
TIME= 1213.199 EXP CONST=0.34252E-02 DEV=-0.18867E-02
TIME= 2017.199 EXP CONST=0.23164E-02 DEV=-0.77791E-03
TIME= 2806.200 EXP CONST=0.21390E-02 DEV=-0.60050E-03
TIME= 3663.000 EXP CONST=0.21059E-02 DEV=-0.56739E-03
TIME= 4276.796 EXP CONST=0.20006E-02 DEV=-0.46210E-03
TIME= 4833.597 EXP CONST=0.19002E-02 DEV=-0.36165E-03
TIME= 5391.000 EXP CONST=0.18693E-02 DEV=-0.33075E-03
TIME= 6066.000 EXP CONST=0.18222E-02 DEV=-0.28371E-03
TIME= 6646.199 EXP CONST=0.17643E-02 DEV=-0.22580E-03
TIME= 7095.000 EXP CONST=0.17893E-02 DEV=-0.25076E-03
TIME= 7838.996 EXP CONST=0.18344E-02 DEV=-0.29592E-03
AVERAGE DEVIATION = 0.74901E-03
STANDARD DEVIATION = 0.35025E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.22254120E-04

CONC OF RCL = 0.01008 CONC OF NAOH = 0.09840
SLOPE = 0.15385E-02LITER/MOLE-SEC CONSTANT= 0.18509E 01
HALF LIFE= 0.471E 04
TIME= 598.200 EXP CONST=0.44835E-02 DEV=-0.29453E-02
TIME= 1213.199 EXP CONST=0.34252E-02 DEV=-0.18867E-02
TIME= 2017.199 EXP CONST=0.23164E-02 DEV=-0.77791E-03
TIME= 2806.200 EXP CONST=0.21390E-02 DEV=-0.60050E-03
TIME= 3663.000 EXP CONST=0.21059E-02 DEV=-0.56739E-03
TIME= 4276.796 EXP CONST=0.20006E-02 DEV=-0.46210E-03
TIME= 4833.597 EXP CONST=0.19002E-02 DEV=-0.36165E-03
TIME= 5391.000 EXP CONST=0.18693E-02 DEV=-0.33075E-03
TIME= 6066.000 EXP CONST=0.18222E-02 DEV=-0.28371E-03
TIME= 6646.199 EXP CONST=0.17643E-02 DEV=-0.22580E-03
TIME= 7095.000 EXP CONST=0.17893E-02 DEV=-0.25076E-03
TIME= 7838.996 EXP CONST=0.18344E-02 DEV=-0.29592E-03
AVERAGE DEVIATION = 0.74901E-03
STANDARD DEVIATION = 0.35025E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.22254120E-04

AVERAGE HALF LIFE= 0.471E 04
AVESLOPE= 0.154E-02

TEMPERATURE IS 35.0 C
DIOXANE-AQ SYSTEM % 30

CONC OF HCL = 0.00980 CONC OF NAOH = 0.09900
SLOPE = 0.15479E-02LITER/MOLE-SEC CONSTANT= 0.19865E 01
HALF LIFE= 0.465E 04
TIME= 643.800 EXP CONST=0.34552E-02 DEV=-0.19973E-02
TIME= 1371.000 EXP CONST=0.29553E-02 DEV=-0.14074E-02
TIME= 1840.199 EXP CONST=0.26736E-02 DEV=-0.11251E-02
TIME= 2346.000 EXP CONST=0.24613E-02 DEV=-0.91340E-03
TIME= 2941.200 EXP CONST=0.22531E-02 DEV=-0.70520E-03
TIME= 3519.999 EXP CONST=0.22463E-02 DEV=-0.69843E-03
TIME= 4150.796 EXP CONST=0.20803E-02 DEV=-0.53242E-03
TIME= 4705.796 EXP CONST=0.20253E-02 DEV=-0.47743E-03
TIME= 5698.199 EXP CONST=0.19096E-02 DEV=-0.36178E-03
TIME= 6496.796 EXP CONST=0.18267E-02 DEV=-0.27885E-03
TIME= 7789.199 EXP CONST=0.18084E-02 DEV=-0.26052E-03
TIME= 8898.000 EXP CONST=0.17251E-02 DEV=-0.17722E-03
AVERAGE DEVIATION = 0.73709E-03
STANDARD DEVIATION = 0.39533E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.25118270E-04

CONC OF HCL = 0.00980 CONC OF NAOH = 0.09900
SLOPE = 0.15413E-02LITER/MOLE-SEC CONSTANT= 0.20123E 01
HALF LIFE= 0.467E 04
TIME= 446.800 EXP CONST=0.32394E-02 DEV=-0.17481E-02
TIME= 1327.800 EXP CONST=0.26556E-02 DEV=-0.11143E-02
TIME= 1903.000 EXP CONST=0.22239E-02 DEV=-0.68261E-03
TIME= 2208.000 EXP CONST=0.25223E-02 DEV=-0.98068E-03
TIME= 2906.999 EXP CONST=0.23446E-02 DEV=-0.80337E-03
TIME= 3487.800 EXP CONST=0.21667E-02 DEV=-0.62540E-03
TIME= 4096.199 EXP CONST=0.20951E-02 DEV=-0.55384E-03
TIME= 4726.199 EXP CONST=0.19211E-02 DEV=-0.43970E-03
TIME= 5707.796 EXP CONST=0.18332E-02 DEV=-0.41193E-03
TIME= 6426.597 EXP CONST=0.19048E-02 DEV=-0.44358E-03
TIME= 7904.796 EXP CONST=0.17543E-02 DEV=-0.21307E-03
TIME= 8953.996 EXP CONST=0.17429E-02 DEV=-0.20151E-03
AVERAGE DEVIATION = 0.75945E-03
STANDARD DEVIATION = 0.58694E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.37483430E-04

AVERAGE HALF LIFE= 0.466E 04
AVESLOPE= 0.154E-02

TEMPERATURE IS 35.0 C
DIOXANE-AQ SYSTEM % 40

CONC OF HCL = 0.01006 CONC OF NAOH = 0.09910
SLOPE = 0.20755E-02LITER/MOLE-SEC CONSTANT= 0.20057E 01
HALF LIFE= 0.347E 04
TIME= 544.800 EXP CONST=0.44933E-02 DEV=-0.24177E-02
TIME= 1021.200 EXP CONST=0.39672E-02 DEV=-0.18916E-02
TIME= 1578.600 EXP CONST=0.35024E-02 DEV=-0.14250E-02
TIME= 1963.799 EXP CONST=0.32668E-02 DEV=-0.11812E-02
TIME= 2479.800 EXP CONST=0.29453E-02 DEV=-0.86972E-03
TIME= 2917.199 EXP CONST=0.26938E-02 DEV=-0.77820E-03
TIME= 3352.800 EXP CONST=0.27199E-02 DEV=-0.64440E-03
TIME= 3953.999 EXP CONST=0.25960E-02 DEV=-0.52046E-03
TIME= 4651.796 EXP CONST=0.24804E-02 DEV=-0.41488E-03
TIME= 5380.796 EXP CONST=0.24269E-02 DEV=-0.35136E-03
TIME= 5977.199 EXP CONST=0.23986E-02 DEV=-0.32329E-03
TIME= 6511.199 EXP CONST=0.23596E-02 DEV=-0.28405E-03
AVERAGE DEVIATION = 0.92532E-03
STANDARD DEVIATION = 0.43629E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.27720990E-04

CONC OF HCL = 0.01011 CONC OF NAOH = 0.09900
SLOPE = 0.20911E-02LITER/MOLE-SEC CONSTANT= 0.17319E 01
HALF LIFE= 0.345E 04
TIME= 562.200 EXP CONST=0.39336E-02 DEV=-0.18425E-02
TIME= 966.000 EXP CONST=0.39107E-02 DEV=-0.18196E-02
TIME= 1534.200 EXP CONST=0.33672E-02 DEV=-0.12761E-02
TIME= 2403.000 EXP CONST=0.29251E-02 DEV=-0.83403E-03
TIME= 2854.200 EXP CONST=0.27604E-02 DEV=-0.66928E-03
TIME= 3292.199 EXP CONST=0.27128E-02 DEV=-0.62166E-03
TIME= 3808.799 EXP CONST=0.25942E-02 DEV=-0.49315E-03
TIME= 4585.199 EXP CONST=0.24761E-02 DEV=-0.33697E-03
TIME= 5017.199 EXP CONST=0.23800E-02 DEV=-0.29703E-03
TIME= 5328.000 EXP CONST=0.24150E-02 DEV=-0.32373E-03
TIME= 5962.796 EXP CONST=0.23496E-02 DEV=-0.25853E-03
TIME= 6491.996 EXP CONST=0.23418E-02 DEV=-0.25069E-03
AVERAGE DEVIATION = 0.75619E-03
STANDARD DEVIATION = 0.45991E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.29157840E-04

AVERAGE HALF LIFE= 0.346E 04
AVESLOPE= 0.208E-02

TEMPERATURE IS 35.0 C
DIOXANE-AQ SYSTEM % 50

CONC OF HCL = 0.01015 CONC OF NAOH = 0.09900
SLOPE = 0.27856E-02LITER/MOLE-SEC CONSTANT= 0.14610E 01
HALF LIFE= 0.259E 04
TIME= 349.800 EXP CONST=0.56014E-02 DEV=-0.29153E-02
TIME= 706.200 EXP CONST=0.50301E-02 DEV=-0.22445E-02
TIME= 949.000 EXP CONST=0.44456E-02 DEV=-0.16603E-02
TIME= 1387.800 EXP CONST=0.39430E-02 DEV=-0.11574E-02
TIME= 1746.599 EXP CONST=0.37009E-02 DEV=-0.91532E-03
TIME= 2108.999 EXP CONST=0.35147E-02 DEV=-0.72900E-03
TIME= 2452.800 EXP CONST=0.33426E-02 DEV=-0.55703E-03
TIME= 2806.799 EXP CONST=0.32977E-02 DEV=-0.51212E-03
TIME= 3406.799 EXP CONST=0.32202E-02 DEV=-0.43462E-03
TIME= 4042.199 EXP CONST=0.31405E-02 DEV=-0.35492E-03
TIME= 4570.199 EXP CONST=0.31351E-02 DEV=-0.34948E-03
TIME= 5185.796 EXP CONST=0.30310E-02 DEV=-0.24544E-03
AVERAGE DEVIATION = 0.99798E-03
STANDARD DEVIATION = 0.38946E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.24745370E-04

CONC OF HCL = 0.01014 CONC OF NAOH = 0.09900
SLOPE = 0.27494E-02LITER/MOLE-SEC CONSTANT= 0.15681E 01
HALF LIFE= 0.262E 04
TIME= 355.200 EXP CONST=0.56726E-02 DEV=-0.29231E-02
TIME= 709.800 EXP CONST=0.50727E-02 DEV=-0.23233E-02
TIME= 1068.199 EXP CONST=0.45940E-02 DEV=-0.18446E-02
TIME= 1395.000 EXP CONST=0.39791E-02 DEV=-0.12297E-02
TIME= 1750.799 EXP CONST=0.36523E-02 DEV=-0.09029E-03
TIME= 2113.799 EXP CONST=0.35536E-02 DEV=-0.80353E-03
TIME= 2461.200 EXP CONST=0.33649E-02 DEV=-0.61548E-03
TIME= 2812.800 EXP CONST=0.33424E-02 DEV=-0.59299E-03
TIME= 3411.000 EXP CONST=0.32129E-02 DEV=-0.46352E-03
TIME= 4053.000 EXP CONST=0.31028E-02 DEV=-0.35337E-03
TIME= 4573.199 EXP CONST=0.31122E-02 DEV=-0.36274E-03
TIME= 5175.000 EXP CONST=0.30258E-02 DEV=-0.27641E-03
AVERAGE DEVIATION = 0.10574E-02
STANDARD DEVIATION = 0.42686E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.26486050E-04

AVERAGE HALF LIFE= 0.260E 04
AVESLOPE= 0.277E-02

TEMPERATURE IS 35.0 C
DIOXANE-AC SYSTEM 2 60

CONC OF RCL = 0.01014 CONC OF NAOH = 0.09900
SLOPE = 0.24311E-02LITER/MOLE-SEC CONSTANT= 0.22637E 01
HALF LIFE= 0.297E 04
TIME= 348.000 EXP CONST=0.[illegible]E-02 DEV=-0.[illegible]E-02
TIME= 726.600 EXP CONST=0.57344E-02 DEV=-0.33032E-02
TIME= 987.000 EXP CONST=0.[illegible]E-02 DEV=-0.[illegible]E-02
TIME= 1275.200 EXP CONST=0.[illegible]E-02 DEV=-0.19155E-02
TIME= 1653.199 EXP CONST=0.[illegible]E-02 DEV=-0.14366E-02
TIME= 1973.999 EXP CONST=0.[illegible]E-02 DEV=-0.12316E-02
TIME= 2416.200 EXP CONST=0.34668E-02 DEV=-0.10857E-02
TIME= 3010.199 EXP CONST=0.32750E-02 DEV=-0.84306E-03
TIME= 3746.999 EXP CONST=0.30443E-02 DEV=-0.65321E-03
TIME= 4413.000 EXP CONST=0.28740E-02 DEV=-0.44297E-03
TIME= 4961.199 EXP CONST=0.28404E-02 DEV=-0.40950E-03
TIME= 5370.000 EXP CONST=0.28462E-02 DEV=-0.41509E-03
AVERAGE DEVIATION = 0.15427E-02
STANDARD DEVIATION = 0.54022E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.34324440E-04

CONC OF RCL = 0.01012 CONC OF NAOH = 0.09900
SLOPE = 0.24189E-02LITER/MOLE-SEC CONSTANT= 0.19517E 01
HALF LIFE= 0.298E 04
TIME= 357.000 EXP CONST=0.63311E-02 DEV=-0.39122E-02
TIME= 709.800 EXP CONST=0.51475E-02 DEV=-0.27285E-02
TIME= 970.800 EXP CONST=0.45497E-02 DEV=-0.21308E-02
TIME= 1234.800 EXP CONST=0.41922E-02 DEV=-0.17733E-02
TIME= 1600.199 EXP CONST=0.37428E-02 DEV=-0.13239E-02
TIME= 2038.799 EXP CONST=0.33616E-02 DEV=-0.94264E-03
TIME= 2454.800 EXP CONST=0.31847E-02 DEV=-0.76577E-03
TIME= 3001.799 EXP CONST=0.31334E-02 DEV=-0.71443E-03
TIME= 3766.799 EXP CONST=0.30195E-02 DEV=-0.60052E-03
TIME= 4451.996 EXP CONST=0.28845E-02 DEV=-0.46561E-03
TIME= 4988.996 EXP CONST=0.27823E-02 DEV=-0.36337E-03
TIME= 5320.796 EXP CONST=0.27216E-02 DEV=-0.30263E-03
AVERAGE DEVIATION = 0.12353E-02
STANDARD DEVIATION = 0.46434E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.29502870E-04

AVERAGE HALF LIFE= 0.297E 04
AVESLOPE= 0.243E-02

TEMPERATURE IS 35.0 C
DIOXANE-AQ SYSTEM % 70

CONC OF RCL = 0.00996 CONC OF NAOH = 0.09900
SLOPE = 0.18610E-02LITER/MOLE-SEC CONSTANT= 0.94851E 00
HALF LIFE= 0.387E 04
TIME= 328.800 EXP CONST=0.49562E-02 DEV=-0.30892E-02
TIME= 693.000 EXP CONST=0.35414E-02 DEV=-0.16804E-02
TIME= 1118.999 EXP CONST=0.28468E-02 DEV=-0.98576E-03
TIME= 1579.200 EXP CONST=0.24595E-02 DEV=-0.59845E-03
TIME= 2018.999 EXP CONST=0.23047E-02 DEV=-0.44363E-03
TIME= 2908.799 EXP CONST=0.21120E-02 DEV=-0.25099E-03
TIME= 3586.200 EXP CONST=0.20944E-02 DEV=-0.23340E-03
TIME= 4335.000 EXP CONST=0.20443E-02 DEV=-0.18323E-03
TIME= 4953.000 EXP CONST=0.20103E-02 DEV=-0.14927E-03
TIME= 5941.199 EXP CONST=0.19923E-02 DEV=-0.13123E-03
TIME= 6811.796 EXP CONST=0.20196E-02 DEV=-0.15859E-03
TIME= 7488.000 EXP CONST=0.20343E-02 DEV=-0.17327E-03
AVERAGE DEVIATION = 0.67311E-03
STANDARD DEVIATION = 0.23867E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.15164550E-04

CONC OF RCL = 0.01001 CONC OF NAOH = 0.09900
SLOPE = 0.20036E-02LITER/MOLE-SEC CONSTANT= 0.82928E 00
HALF LIFE= 0.360E 04
TIME= 337.200 EXP CONST=0.53563E-02 DEV=-0.33524E-02
TIME= 714.600 EXP CONST=0.36075E-02 DEV=-0.16840E-02
TIME= 1144.800 EXP CONST=0.28748E-02 DEV=-0.87115E-03
TIME= 1567.800 EXP CONST=0.25570E-02 DEV=-0.55338E-03
TIME= 2041.799 EXP CONST=0.22208E-02 DEV=-0.22419E-03
TIME= 2917.199 EXP CONST=0.21106E-02 DEV=-0.11403E-03
TIME= 3589.800 EXP CONST=0.21956E-02 DEV=-0.19934E-03
TIME= 4338.000 EXP CONST=0.21461E-02 DEV=-0.14984E-03
TIME= 5025.000 EXP CONST=0.21233E-02 DEV=-0.12705E-03
TIME= 5992.796 EXP CONST=0.21036E-02 DEV=-0.10737E-03
TIME= 6825.000 EXP CONST=0.21119E-02 DEV=-0.11568E-03
TIME= 7566.000 EXP CONST=0.22144E-02 DEV=-0.21792E-03
AVERAGE DEVIATION = 0.68[illegible]E-03
STANDARD DEVIATION = 0.47[illegible]E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.[illegible]E-04

AVERAGE HALF LIFE= 0.373E 04
AVESLOPE= 0.193E-02

TEMPERATURE IS 40.0 C
DIOXANE-AQ SYSTEM = 30

CONC OF HCL = 0.00987 CONC OF NAOH = 0.09880
SLOPE = 0.22614E-02LITER/MOLE-SEC CONSTANT= 0.19892E 01
HALF LIFE= 0.319E 04
TIME= 463.800 EXP CONST=0.51840E-02 DEV=-0.29226E-02
TIME= 931.800 EXP CONST=0.43419E-02 DEV=-0.20805E-02
TIME= 1456.200 EXP CONST=0.37591E-02 DEV=-0.14977E-02
TIME= 1909.200 EXP CONST=0.34654E-02 DEV=-0.12040E-02
TIME= 2391.000 EXP CONST=0.32052E-02 DEV=-0.93877E-03
TIME= 2869.200 EXP CONST=0.30282E-02 DEV=-0.76179E-03
TIME= 3376.799 EXP CONST=0.29163E-02 DEV=-0.65035E-03
TIME= 3931.799 EXP CONST=0.28976E-02 DEV=-0.63161E-03
TIME= 4321.199 EXP CONST=0.27209E-02 DEV=-0.45445E-03
TIME= 4868.996 EXP CONST=0.26892E-02 DEV=-0.42268E-03
TIME= 5490.000 EXP CONST=0.25827E-02 DEV=-0.32126E-03
TIME= 5893.796 EXP CONST=0.25798E-02 DEV=-0.31834E-03
AVERAGE DEVIATION = 0.10023E-02
STANDARD DEVIATION = 0.49256E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.31295030E-04

CONC OF HCL = 0.00988 CONC OF NAOH = 0.09880
SLOPE = 0.23332E-02LITER/MOLE-SEC CONSTANT= 0.19548E 01
HALF LIFE= 0.309E 04
TIME= 486.600 EXP CONST=0.52115E-02 DEV=-0.29784E-02
TIME= 952.800 EXP CONST=0.43744E-02 DEV=-0.20413E-02
TIME= 1496.200 EXP CONST=0.37649E-02 DEV=-0.14317E-02
TIME= 1930.799 EXP CONST=0.35180E-02 DEV=-0.11846E-02
TIME= 2426.999 EXP CONST=0.32130E-02 DEV=-0.88795E-03
TIME= 2916.000 EXP CONST=0.30494E-02 DEV=-0.71459E-03
TIME= 3409.200 EXP CONST=0.29169E-02 DEV=-0.58215E-03
TIME= 3885.000 EXP CONST=0.27723E-02 DEV=-0.43913E-03
TIME= 4354.796 EXP CONST=0.26219E-02 DEV=-0.28873E-03
TIME= 4933.796 EXP CONST=0.27507E-02 DEV=-0.41754E-03
TIME= 5506.199 EXP CONST=0.24722E-02 DEV=-0.13904E-03
TIME= 5923.000 EXP CONST=0.26230E-02 DEV=-0.28990E-03
AVERAGE DEVIATION = 0.97427E-03
STANDARD DEVIATION = 0.43513E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.27644650E-04

AVERAGE HALF LIFE= 0.314E 04
AVESLOPE= 0.230E-02

TEMPERATURE IS 40.0 C
DIOXANE-AQ SYSTEM % 40

CONC OF HCL = 0.01009 CONC OF NAOH = 0.09880
SLOPE = -0.28041E-02LITER/MOLE-SEC CONSTANT= 0.14961E 01
HALF LIFE= 0.258E 04
TIME= 348.000 EXP CONST=0.56509E-02 DEV=-0.28557E-02
TIME= 690.000 EXP CONST=0.50739E-02 DEV=-0.22698E-02
TIME= 1000.199 EXP CONST=0.44986E-02 DEV=-0.16845E-02
TIME= 1381.699 EXP CONST=0.40142E-02 DEV=-0.12107E-02
TIME= 1746.000 EXP CONST=0.37347E-02 DEV=-0.93064E-03
TIME= 2106.000 EXP CONST=0.35321E-02 DEV=-0.72802E-03
TIME= 2454.600 EXP CONST=0.34123E-02 DEV=-0.60816E-03
TIME= 2801.400 EXP CONST=0.32373E-02 DEV=-0.43319E-03
TIME= 3403.599 EXP CONST=0.33305E-02 DEV=-0.52639E-03
TIME= 4045.199 EXP CONST=0.32157E-02 DEV=-0.41164E-03
TIME= 4566.000 EXP CONST=0.31360E-02 DEV=-0.33191E-03
TIME= 5182.796 EXP CONST=0.30326E-02 DEV=-0.22848E-03
AVERAGE DEVIATION = 0.10183E-02
STANDARD DEVIATION = 0.48864E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.31046960E-04

CONC OF HCL = 0.01009 CONC OF NAOH = 0.09880
SLOPE = -0.27964E-02LITER/MOLE-SEC CONSTANT= 0.15394E 01
HALF LIFE= 0.258E 04
TIME= 354.000 EXP CONST=0.57350E-02 DEV=-0.29386E-02
TIME= 708.600 EXP CONST=0.51014E-02 DEV=-0.23050E-02
TIME= 1068.000 EXP CONST=0.47093E-02 DEV=-0.19129E-02
TIME= 1398.000 EXP CONST=0.40453E-02 DEV=-0.12489E-02
TIME= 1748.999 EXP CONST=0.36553E-02 DEV=-0.85485E-03
TIME= 2113.799 EXP CONST=0.35971E-02 DEV=-0.80709E-03
TIME= 2460.599 EXP CONST=0.33490E-02 DEV=-0.59258E-03
TIME= 2811.000 EXP CONST=0.33400E-02 DEV=-0.56361E-03
TIME= 3408.000 EXP CONST=0.32331E-02 DEV=-0.43666E-03
TIME= 4050.000 EXP CONST=0.31064E-02 DEV=-0.30994E-03
TIME= 4570.199 EXP CONST=0.31264E-02 DEV=-0.33003E-03
TIME= 5178.000 EXP CONST=0.31232E-02 DEV=-0.32675E-03
AVERAGE DEVIATION = 0.10487E-02
STANDARD DEVIATION = 0.46230E-04
AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.29411730E-04

AVERAGE HALF LIFE= 0.258E 04
AVESLOPE= 0.280E-02

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TEMPERATURE IS  40.0 C
DIOXANE-AQ SYSTEM % 50

CONC OF RCL = 0.01010      CONC OF NAOH = 0.09880
 SLOPE =  0.33780E-02LITER/MOLE-SEC      CONSTANT=  0.17729E 01
 HALF LIFE=      0.214E 04
 TIME=     339.000   EXP CONST=0.71014E-02   DEV=-0.37234E-02
 TIME=     610.800   EXP CONST=0.42888E-02   DEV=-0.29108E-02
 TIME=     964.800   EXP CONST=0.53583E-02   DEV=-0.19803E-02
 TIME=    1399.200   EXP CONST=0.47343E-02   DEV=-0.13559E-02
 TIME=    1620.000   EXP CONST=0.45115E-02   DEV=-0.11335E-02
 TIME=    1916.999   EXP CONST=0.44421E-02   DEV=-0.10641E-02
 TIME=    2230.199   EXP CONST=0.42142E-02   DEV=-0.83615E-03
 TIME=    2533.199   EXP CONST=0.40685E-02   DEV=-0.69051E-03
 TIME=    2800.799   EXP CONST=0.40205E-02   DEV=-0.64254E-03
 TIME=    3446.999   EXP CONST=0.40000E-02   DEV=-0.62203E-03
 TIME=    4015.199   EXP CONST=0.37628E-02   DEV=-0.38481E-03
 TIME=    4335.000   EXP CONST=0.37153E-02   DEV=-0.33726E-03
 AVERAGE DEVIATION =  0.13068E-02
 STANDARD DEVIATION =  0.60173E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.38232070E-04

CONC OF RCL = 0.01001      CONC OF NAOH = 0.09880
 SLOPE =  0.34917E-02LITER/MOLE-SEC      CONSTANT=  0.12403E 01
 HALF LIFE=      0.207E 04
 TIME=     295.800   EXP CONST=0.67382E-02   DEV=-0.32465E-02
 TIME=     586.800   EXP CONST=0.57765E-02   DEV=-0.22849E-02
 TIME=     934.200   EXP CONST=0.50484E-02   DEV=-0.15568E-02
 TIME=    1306.799   EXP CONST=0.45039E-02   DEV=-0.10122E-02
 TIME=    1696.200   EXP CONST=0.44891E-02   DEV=-0.99744E-03
 TIME=    1855.199   EXP CONST=0.41104E-02   DEV=-0.61916E-03
 TIME=    2164.200   EXP CONST=0.40502E-02   DEV=-0.55894E-03
 TIME=    2441.999   EXP CONST=0.39344E-02   DEV=-0.44329E-03
 TIME=    2833.199   EXP CONST=0.38433E-02   DEV=-0.35238E-03
 TIME=    3382.800   EXP CONST=0.37763E-02   DEV=-0.28556E-03
 TIME=    3964.200   EXP CONST=0.37302E-02   DEV=-0.24755E-03
 TIME=    4225.796   EXP CONST=0.36918E-02   DEV=-0.42716E-03
 AVERAGE DEVIATION =  0.10033E-02
 STANDARD DEVIATION =  0.47727E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.48931770E-04

 AVERAGE HALF LIFE=      0.210E 04
 AVESLOPE=     0.343E-02
```

```
TEMPERATURE IS  40.0 C
DIOXANE-AQ SYSTEM % 60

CONC OF HCL = 0.01011        CONC OF NAOH = 0.00880
 SLOPE =  0.29306E-02LITER/MOLE-SEC      CONSTANT=  0.13914E 01
 HALF LIFE=      0.24EE 04
 TIME=     293.800   EXP CONST=0.441095E-02   DEV=-0.36803E-02
 TIME=     549.000   EXP CONST=0.539560E-02   DEV=-0.24645E-02
 TIME=     862.800   EXP CONST=0.458135E-02   DEV=-0.16509E-02
 TIME=    1177.800   EXP CONST=0.416245E-02   DEV=-0.12319E-02
 TIME=    1466.999   EXP CONST=0.401950E-02   DEV=-0.10893E-02
 TIME=    1720.799   EXP CONST=0.415888E-02   DEV=-0.12293E-02
 TIME=    2314.200   EXP CONST=0.346116E-02   DEV=-0.47117E-03
 TIME=    2767.800   EXP CONST=0.330726E-02   DEV=-0.32765E-03
 TIME=    3283.199   EXP CONST=0.332546E-02   DEV=-0.39486E-03
 TIME=    3781.799   EXP CONST=0.321216E-02   DEV=-0.28155E-03
 TIME=    4313.996   EXP CONST=0.323126E-02   DEV=-0.30060E-03
 TIME=    4885.796   EXP CONST=0.328426E-02   DEV=-0.35360E-03
 AVERAGE DEVIATION =   0.112609E-02
 STANDARD DEVIATION =   0.700005E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.44479130E-04

CONC OF HCL = 0.01011        CONC OF NAOH = 0.00880
 SLOPE =  0.29743E-02LITER/MOLE-SEC      CONSTANT=  0.13216E 01
 HALF LIFE=      0.243E 04
 TIME=     304.200   EXP CONST=0.641245E-02   DEV=-0.34381E-02
 TIME=     586.800   EXP CONST=0.528538E-02   DEV=-0.23110E-02
 TIME=     870.000   EXP CONST=0.464497E-02   DEV=-0.16755E-02
 TIME=    1150.199   EXP CONST=0.439556E-02   DEV=-0.14213E-02
 TIME=    1433.199   EXP CONST=0.392558E-02   DEV=-0.95149E-03
 TIME=    1804.200   EXP CONST=0.369360E-02   DEV=-0.72449E-03
 TIME=    2257.800   EXP CONST=0.355778E-02   DEV=-0.58345E-03
 TIME=    2778.000   EXP CONST=0.338689E-02   DEV=-0.41462E-03
 TIME=    3248.999   EXP CONST=0.330466E-02   DEV=-0.33023E-03
 TIME=    3757.800   EXP CONST=0.331615E-02   DEV=-0.34182E-03
 TIME=    4324.199   EXP CONST=0.326155E-02   DEV=-0.28719E-03
 TIME=    4881.000   EXP CONST=0.329376E-02   DEV=-0.32331E-03
 AVERAGE DEVIATION =   0.106659E-02
 STANDARD DEVIATION =   0.381165E-04
 AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.24217760E-04

AVERAGE HALF LIFE=      0.245E 04
AVESLOPE=     0.295E-02
```

```
TEMPERATURE IS  40.0 C
DIOXANE-AQ SYSTEM % 70

CONC OF RCL = 0.01010      CONC OF NAOH = 0.09880
 SLOPE =  0.25309E-02LITER/MOLE-SEC      CONSTANT=  0.21833E 01
 HALF LIFE=    0.285E 04
 TIME=    349.200  EXP CONST=0.69097E-02  DEV=-0.43738E-02
 TIME=    705.000  EXP CONST=0.57230E-02  DEV=-0.31921E-02
 TIME=    988.200  EXP CONST=0.49161E-02  DEV=-0.23852E-02
 TIME=   1279.000  EXP CONST=0.44182E-02  DEV=-0.18873E-02
 TIME=   1725.000  EXP CONST=0.36670E-02  DEV=-0.11360E-02
 TIME=   1972.800  EXP CONST=0.37157E-02  DEV=-0.11848E-02
 TIME=   2418.000  EXP CONST=0.35732E-02  DEV=-0.10423E-02
 TIME=   3008.999  EXP CONST=0.33331E-02  DEV=-0.80213E-03
 TIME=   3746.999  EXP CONST=0.31048E-02  DEV=-0.57385E-03
 TIME=   4417.199  EXP CONST=0.30363E-02  DEV=-0.50535E-03
 TIME=   4986.000  EXP CONST=0.29897E-02  DEV=-0.45879E-03
 TIME=   5359.796  EXP CONST=0.28575E-02  DEV=-0.32659E-03
  AVERAGE DEVIATION =   0.14894E-02
  STANDARD DEVIATION =   0.54444E-04
  AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.34592470E-04

 CONC OF RCL = 0.01012      CONC OF NAOH = 0.09880
 SLOPE =  0.24616E-02LITER/MOLE-SEC      CONSTANT=  0.19719E 01
 HALF LIFE=    0.293E 04
 TIME=    366.000  EXP CONST=0.67567E-02  DEV=-0.42951E-02
 TIME=    712.200  EXP CONST=0.52455E-02  DEV=-0.27839E-02
 TIME=    981.000  EXP CONST=0.46031E-02  DEV=-0.21415E-02
 TIME=   1237.199  EXP CONST=0.42775E-02  DEV=-0.18159E-02
 TIME=   1600.799  EXP CONST=0.37728E-02  DEV=-0.13112E-02
 TIME=   2036.999  EXP CONST=0.335[illegible]E-02  DEV=-0.[illegible]E-03
 TIME=   2433.000  EXP CONST=0.31[illegible]E-02  DEV=-0.7[illegible]E-03
 TIME=   3006.000  EXP CONST=0.31[illegible]E-02  DEV=-0.727[illegible]E-03
 TIME=   3766.799  EXP CONST=0.30343E-02  DEV=-0.5777[illegible]E-03
 TIME=   4455.000  EXP CONST=0.29471E-02  DEV=-0.4[illegible]E-03
 TIME=   4990.799  EXP CONST=0.2[illegible]E-02  DEV=-0.37437E-03
 TIME=   5332.795  EXP CONST=0.27[illegible]E-02  DEV=-0.32143E-03
  AVERAGE DEVIATION =   0.127[illegible]E-02
  STANDARD DEVIATION =   0.47[illegible]E-04
  AT 95% CONFIDENCE LIMIT K=SLOPE+(OR -)0.2[illegible]E-04

 AVERAGE HALF LIFE=     0.2[illegible]E 04
 AVESLOPE=     0.25[illegible]E-02
```

```
FORMAT (6X,9HDIOXANE %,I3)
FORMAT (1X,15HTEMPERATURE IS,F6.1,1X,1HC)
FORMAT (2X,13HACT. ENERGY =,F14.5,8HCAL/MOLE)
FORMAT (2X,14HHEAT OF ACT. =,F14.5,1X,8HCAL/MALE)
END
  293.16          298.16          303.16          308.16          313.16
1.38E-23      6.6252E-24           1.987
0.000564        0.000724        0.001090        0.001540        0.002300
0.000901        0.001190        0.001520        0.002080        0.002900
0.001140        0.001300        0.002040        0.002770        0.003430
0.001050        0.001270        0.001620        0.002430        0.002950
0.000990        0.001050        0.001540        0.001930        0.002500
```

```
          /DATA
      DIOXANE % 30
 SLOPE =   -0.65378E 04      LN A =   0.14758E 02
 ACT. ENERGY =    0.12991E 05CAL/MOLE


TEMPERATURE IS,   20.0 C
 HEAT OF ACT. =    0.12408E 05 CAL/MALE
 ENTROPY =    0.14716E 02CAL/MOLE-DEG
 FREE ENERGY =    0.80939E 04CAL/MOLE

TEMPERATURE IS,   25.0 C
 HEAT OF ACT. =    0.12398E 05 CAL/MALE
 ENTROPY =    0.14436E 02CAL/MOLE-DEG
 FREE ENERGY =    0.80941E 04CAL/MOLE

TEMPERATURE IS,   30.0 C
 HEAT OF ACT. =    0.12388E 05 CAL/MALE
 ENTROPY =    0.14497E 02CAL/MOLE-DEG
 FREE ENERGY =    0.79933E 04CAL/MOLE

TEMPERATURE IS,   35.0 C
 HEAT OF ACT. =    0.12378E 05 CAL/MALE
 ENTROPY =    0.14456E 02CAL/MOLE-DEG
 FREE ENERGY =    0.79236E 04CAL/MOLE

TEMPERATURE IS,   40.0 C
 HEAT OF ACT. =    0.12368E 05 CAL/MALE
 ENTROPY =    0.14548E 02CAL/MOLE-DEG
 FREE ENERGY =    0.78126E 04CAL/MOLE


      DIOXANE % 40
 SLOPE =   -0.51819E 04      LN A =   0.10644E 02
 ACT. ENERGY =    0.10296E 05CAL/MOLE


TEMPERATURE IS,   20.0 C
 HEAT OF ACT. =    0.97139E 04 CAL/MALE
 ENTROPY =    0.64567E 01CAL/MOLE-DEG
 FREE ENERGY =    0.78211E 04CAL/MOLE

TEMPERATURE IS,   25.0 C
 HEAT OF ACT. =    0.97040E 04 CAL/MALE
 ENTROPY =    0.63869E 01CAL/MOLE-DEG
 FREE ENERGY =    0.77996E 04CAL/MOLE

TEMPERATURE IS,   30.0 C
 HEAT OF ACT. =    0.96940E 04 CAL/MALE
 ENTROPY =    0.62706E 01CAL/MOLE-DEG
 FREE ENERGY =    0.77930E 04CAL/MOLE

TEMPERATURE IS,   35.0 C
```

HEAT OF ACT. = 0.96841E 04 CAL/MALE
ENTROPY = 0.63103E 01CAL/MOLE-DEG
FREE ENERGY = 0.77395E 04CAL/MOLE

TEMPERATURE IS, 40.0 C
HEAT OF ACT. = 0.96742E 04 CAL/MALE
ENTROPY = 0.63355E 01CAL/MOLE-DEG
FREE ENERGY = 0.76901E 04CAL/MOLE

DIOXANE % 50
SLOPE = -0.54331E 04 LN A = 0.11694E 02
ACT. ENERGY = 0.10796E 05CAL/MOLE

TEMPERATURE IS, 20.0 C
HEAT OF ACT. = 0.10213E 05 CAL/MALE
ENTROPY = 0.86266E 01CAL/MOLE-DEG
FREE ENERGY = 0.76340E 04CAL/MOLE

TEMPERATURE IS, 25.0 C
HEAT OF ACT. = 0.10203E 05 CAL/MALE
ENTROPY = 0.82365E 01CAL/MOLE-DEG
FREE ENERGY = 0.77473E 04CAL/MOLE

TEMPERATURE IS, 30.0 C
HEAT OF ACT. = 0.10193E 05 CAL/MALE
ENTROPY = 0.85016E 01CAL/MOLE-DEG
FREE ENERGY = 0.76158E 04CAL/MOLE

TEMPERATURE IS, 35.0 C
HEAT OF ACT. = 0.10183E 05 CAL/MALE
ENTROPY = 0.84991E 01CAL/MOLE-DEG
FREE ENERGY = 0.75641E 04CAL/MOLE

TEMPERATURE IS, 40.0 C
HEAT OF ACT. = 0.10173E 05 CAL/MALE
ENTROPY = 0.83324E 01CAL/MOLE-DEG
FREE ENERGY = 0.75639E 04CAL/MOLE

DIOXANE % 60
SLOPE = -0.49805E 04 LN A = 0.10077E 02
ACT. ENERGY = 0.99963E 04CAL/MOLE

TEMPERATURE IS, 20.0 C
HEAT OF ACT. = 0.93138E 04 CAL/MALE
ENTROPY = 0.53961E 01CAL/MOLE-DEG
FREE ENERGY = 0.77319E 04CAL/MOLE

TEMPERATURE IS, 25.0 C
HEAT OF ACT. = 0.93039E 04 CAL/MALE
ENTROPY = 0.51744E 01CAL/MOLE-DEG
FREE ENERGY = 0.77611E 04CAL/MOLE

TEMPERATURE IS, 30.0 C

HEAT OF ACT. = 0.92940E 04 CAL/MALE
ENTROPY = 0.50776E 01CAL/MOLE-DEG
FREE ENERGY = 0.77546E 04CAL/MOLE

TEMPERATURE IS, 35.0 C
HEAT OF ACT. = 0.92840E 04 CAL/MALE
ENTROPY = 0.53216E 01CAL/MOLE-DEG
FREE ENERGY = 0.76443E 04CAL/MOLE

TEMPERATURE IS, 40.0 C
HEAT OF ACT. = 0.92741E 04 CAL/MALE
ENTROPY = 0.51616E 01CAL/MOLE-DEG
FREE ENERGY = 0.76577E 04CAL/MOLE

DIOXANE % 70
SLOPE = -0.49504E 04 LN A = 0.93126E 01
ACT. ENERGY = 0.98364E 04CAL/MOLE

TEMPERATURE IS, 20.0 C
HEAT OF ACT. = 0.92539E 04 CAL/MALE
ENTROPY = 0.48408E 01CAL/MOLE-DEG
FREE ENERGY = 0.78348E 04CAL/MOLE

TEMPERATURE IS, 25.0 C
HEAT OF ACT. = 0.92440E 04 CAL/MALE
ENTROPY = 0.45955E 01CAL/MOLE-DEG
FREE ENERGY = 0.78738E 04CAL/MOLE

TEMPERATURE IS, 30.0 C
HEAT OF ACT. = 0.92341E 04 CAL/MALE
ENTROPY = 0.47784E 01CAL/MOLE-DEG
FREE ENERGY = 0.77852E 04CAL/MOLE

TEMPERATURE IS, 35.0 C
HEAT OF ACT. = 0.92241E 04 CAL/MALE
ENTROPY = 0.46689E 01CAL/MOLE-DEG
FREE ENERGY = 0.77853E 04CAL/MOLE

TEMPERATURE IS, 40.0 C
HEAT OF ACT. = 0.92142E 04 CAL/MALE
ENTROPY = 0.46415E 01CAL/MOLE-DEG
FREE ENERGY = 0.77607E 04CAL/MOLE

Figure 4

PLOT OF THE SECOND-ORDER RATE CONSTANT ON A LOGARITHIM SCALE *VS.* 1/T FOR DETERMINATION OF ARRHENIUS ACTIVATION PARAMETERS

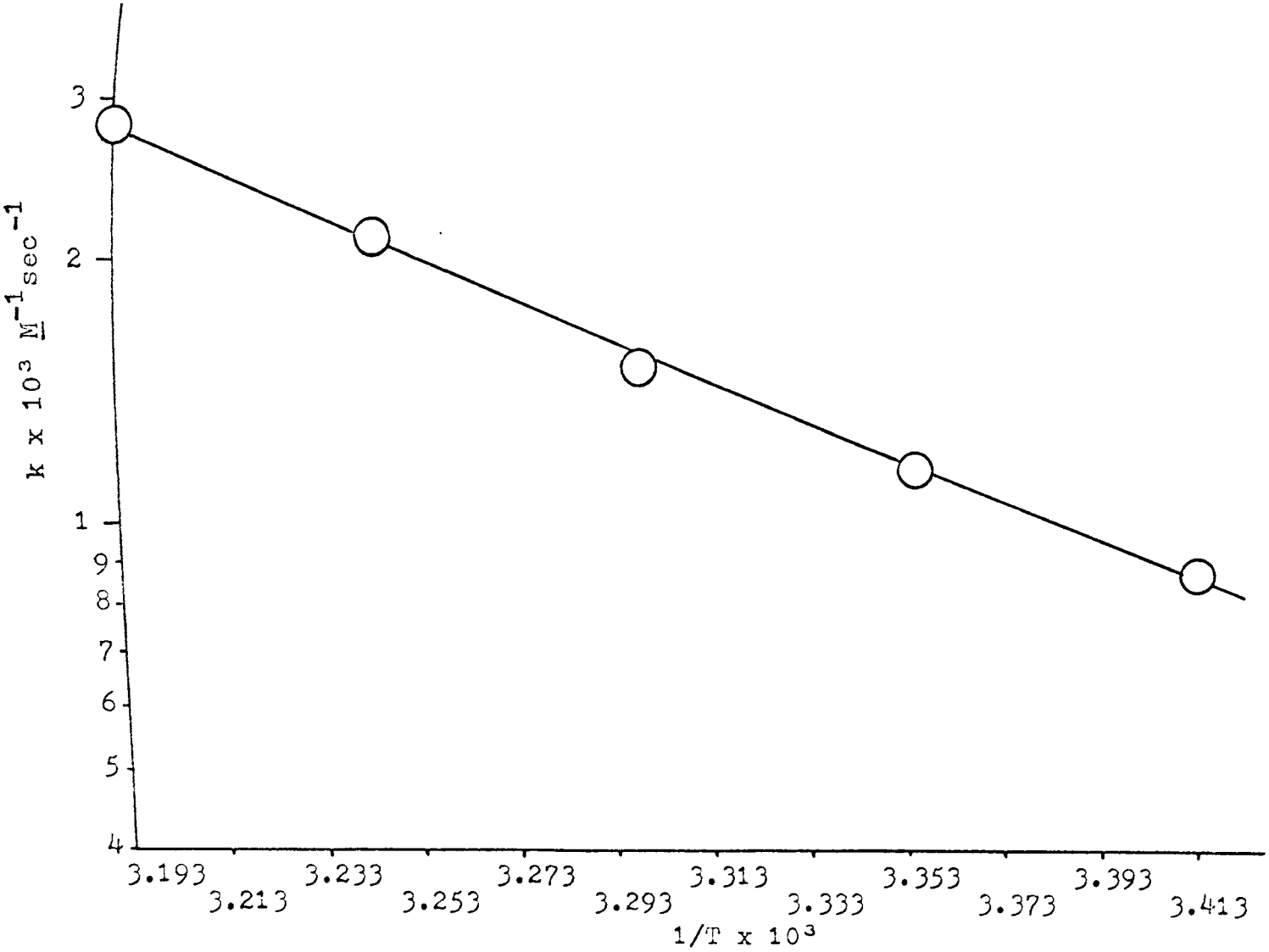
k x 10³ M⁻¹sec⁻¹
3
2
1
9
8
7
6
5
4
3.193
3.213
3.233
3.253
3.273
3.293
3.313
3.333
3.353
3.373
3.393
3.413
1/T x 10³

Figure 4

APPENDIX II

THE APPLICATION OF AKERLOF'S EMPERICAL EQUATION FOR THE INTERPOLATION OF DIELECTRIC CONSTANT

The equation employed by Åkerlöf[10],

$$\log \mathcal{E} = \log a - bt$$

(a and b are empirical constants, and t is temperature in C) has been used to calculate the dielectric constant of the solvent mixtures at various temperatures.

The curves of log a and b vs. wt.% of dioxane in Figure 5 are constructed by using the table from Akerlof (shown below) and used for the interpolation of log a and b which are specific to the wt.% of dioxane for this experiment.

Dioxane, wt.%	log a	b
0	1.9461	0.00205
10	1.8969	.00215
20	1.8398	.00224
30	1.7734	.00233
40	1.6935	.00241
50	1.5965	.00247
60	1.4747	.00249
70	1.3090	.00245
80	1.0860	.00225
90	0.7896	.00164
95	.5923	.00100
100	.3234	.00004

The results of the interpolation log a and b are also listed down below:

Dioxane, vol.%	Dioxane, wt.%	log a	b x 10^3
30	29.94	1.773	2.325
40	41.61	1.685	2.417
50	50.76	1.593	2.471
60	62.29	1.495	2.487
70	70.64	1.303	2.445

The log a and b reading from the curves in Figure 5 are substituted into the Akerlof's empirical equation to calculate the dielectric constant, $\mathcal{E}$, of the solvent mixtures at different temperature, as in Table II:

TABLE II INTERPOLATED VALUES FOR THE DIELECTRIC CONSTANTS OF A SERIES DIOXANE-WATER MIXTURES AT VARIOUS TEMPERATURES

	Dioxane wt.%				
°C	29.94	41.61	50.76	62.29	70.64
20	53.27	43.32	34.96	27.88	17.95
25	51.86	42.15	33.98	27.09	17.45
30	50.50	40.97	33.03	26.33	16.97
35	48.60	39.85	32.10	25.58	16.50
40	47.86	38.75	31.20	24.86	16.04

Figure 5

PLOT OF WEIGHT PERCENTAGE OF DIOXANE-WATER IXTURES VS. AKERLOF'S EMPIRICAL CONSTANTS log a AND b FOR THE INTERPOLATION OF DIELECTRIC CONSTANT

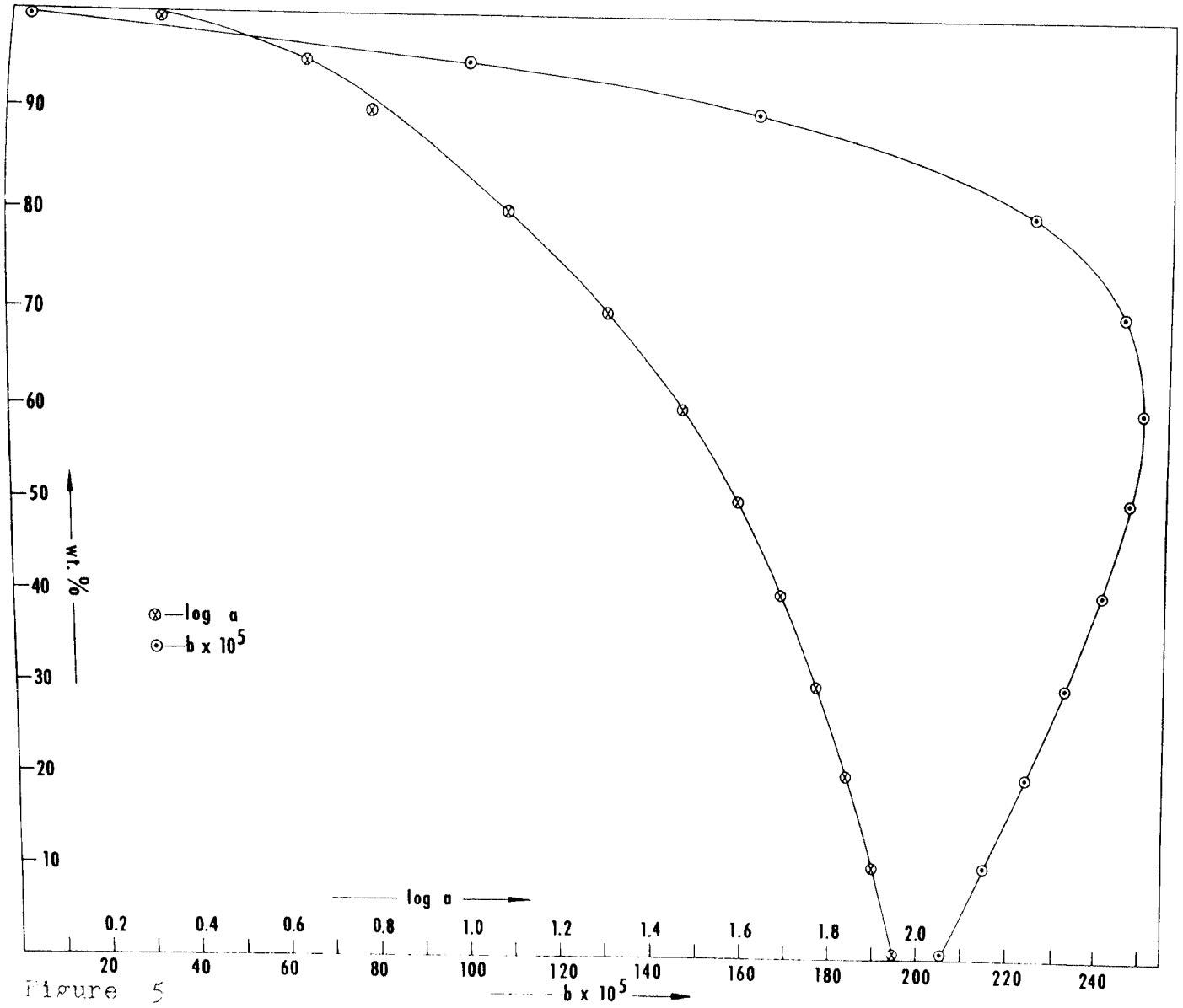
90
80
70
60
50
40
30
20
10
wt. %
⊗—log a
⊙—b x 10^5
log a
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
20
40
60
80
100
120
140
160
180
200
220
240
b x 10^5

Figure 5

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VI. VITA

The author was born to Mr. and Mrs. Shih-Lung Ho on August 6, 1935, in Canton, China, and was married to Miss Wen-Huei Kao on June 3, 1967 in Ames, Iowa, U.S.A.. He received his primary education at home under his parents' teaching in Chinese classic literature and received his secondary education in Shin-Chu, Taiwan, China. He has received his college education in Tunghai University, Taichung, Taiwan, China and received a Bachelor of Science Degree in Chemistry in June, 1959. He came to the United States and enrolled in the Graduate School of the University of Missouri at Rolla in September 1965, and has held the AVCO Fellowship for the period September, 1965 to January 1968, and the Department Research Assistantship for the period February 1968 to June 1968.

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