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KINETIC MODELING STUDY OF
CATALYTIC HYDROGENATION OF CODIMER

BY

WILLIAM MOUNCE

A THESIS
PRESENTED IN PARTIAL FULFILLMENT OF
THE REQUIREMENTS FOR THE DEGREE
OF
MASTER OF SCIENCE IN CHEMICAL ENGINEERING
AT
NEWARK COLLEGE OF ENGINEERING

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Newark, New Jersey

1973

ABSTRACT

A kinetic modeling study was made on a gas phase catalytic reaction. The data used was that on the hydrogenation of codimer, collected by Tschernitz, et al. The objective was to determine if non-linear least squares regression offers an advantage over linear least squares regression in discriminating between Langmuir-Hinshelwood kinetic equations.

For the experimental data in question, it was found that neither linear nor non-linear regression could distinguish between the two plausible mechanisms. With the particular mechanistic equations and range of data used in this study, the more laborious non-linear analysis offered no advantage over linear regression in discriminating between the two plausible mechanisms in question.

By the use of synthetic data with error introduced, it was found that neither the linear nor the non-linear technique introduced any additional error.

The experimental data were also fitted to a non-theoretical exponential form of equation. The fit with this form was essentially just as good as with the two best theoretical equations. This suggests that the simpler form of equation would be just as suitable for design work.

APPROVAL OF THESIS

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Newark, New Jersey
May, 1973

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INTRODUCTION

The first objective of this study was to determine the usefulness of non-linear regression for selecting the correct kinetic mechanism for catalytic gas phase reactions. In particular it was desired to determine if non-linear regression is able to provide a better fit for kinetic data than linear regression, as has been reported by others.

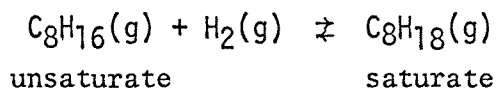
Kittrel, Mezaki, and Watson(8) reported that non-linear least squares gave a better fit to experimental data than linear least squares. The reaction studied was the oxidation of methane over a palladium-alumina catalyst. The sum of residual squares was reduced from 7.2×10^{-6} with linear least squares to 1.1×10^{-10} using a non-linear fit.

Kittrel, Hunter and Watson (7) treated data on the reaction of nitric oxide and hydrogen over a copper, zinc, chromia catalyst. They reported that non-linear regression gave a slightly better fit than the linear regression. For the model showing the best fit, the sum of residual squares was reduced from 5.0×10^{-11} to 3.1×10^{-11} . They stated that the advantage of non-linear analysis over linear analysis could become more important with other Hougen-Watson models and other sets of data.

Lapidus and Peterson (9) studied data on dehydration of ethanol to diethyl ether and water. They found that non-linear regression

was a useful tool for fitting the data. However, they did not conclude whether there was a clear advantage over linear regression in discriminating between mechanisms.

The reaction system chosen for the present study was the hydrogenation of mixed isooctene (codimer) over a supported nickel catalyst. The experimental data are due to Tschernitz, Bornstein, Beckmann, and Hougen(10). The reaction is as follows:



The experiments were carried out in a short tubular reactor designed to approximate a differential reactor. The experimental program involved varying the partial pressure of each of the three components over a range of 0.1 to 2.6 atmospheres. Three sets of data were collected - at 200°C, 275°C and 325°C. Under the conditions of the experiments it was known that the effect of diffusional resistance was negligible. It was also established that the extent of the reverse reaction was negligible at the temperatures used.

Tschernitz, et al. considered eighteen possible theoretical mechanisms. The data were analyzed by linear least squares regression. They used the values of the parameters obtained as the criterion for accepting or rejecting a particular mechanism. If any of the adsorption constants or the reaction rate constant was negative,

the mechanism was rejected. Likewise, if any of the parameters were non-zero when they should have been zero, the mechanism was rejected. Only mechanisms (d) and (h) met these criteria. These two plausible mechanisms and their respective Langmuir-Hinshelwood kinetic equations are given below. Tschernitz, et al, reported that the average residual error was $\pm 17\%$ for mechanism (d) and $\pm 34\%$ for mechanism (h). On this basis they selected (d) as the correct model.

Mechanism (d) - Reaction rate controlling with molecularly adsorbed hydrogen

$$r = \frac{E_k K_H K_U (P_H P_U - P_S / K_e)}{(1 + K_H K_U + K_U P_U + K_S P_S)^2}$$

Mechanism (h) - Reaction rate controlling with atomically adsorbed hydrogen

$$r = \frac{E_k K_H K_U (P_H P_U - P_S / K_e)}{(1 + \sqrt{K_H P_H} + K_U P_U + K_S P_S)^3}$$

Chou (3) has correctly pointed out that from a statistical viewpoint the criteria used by Tschernitz, et al, are not sufficient to reject a model. The confidence interval of the parameters as determined by regression must be considered. For instance, a parameter may have a non-zero value by linear regression. Yet, a value of zero may fall within the 95% confidence region of the parameter.

Blakemore and Hoerl (2) made a regression study of the subject data. They used the measured change in the refractive index of the oil as the dependent variable, rather than the calculated reaction rate. They fitted all the equations to the data by linear regression. They found that mechanisms (d) and (h) gave the best fit, confirming one conclusion of Tschernitz, et al. Their quantitative results are not directly comparable with Tschernitz, et al, because Blakemore and Hoerl used a different dependent variable and reported sums of residual squares only, not percent error. However, they found significantly higher residual variance at 275°C with mechanism (h). When they used non-linear regression, the difference at 275°C was eliminated. The fit of the two mechanisms became indistinguishable.

In the present study the data generated by Tschernitz, et al, were fitted to the two plausible mechanisms by linear and non-linear least squares regression. The basis of discrimination was the average percent error.

A second objective of this study was to investigate the closeness of fit of a non-catalytic, exponential form of equation and compare its fit to that of the theoretical Langmuir-Hinshelwood equations. Weller (11) has suggested that gas phase kinetic data can be fitted to an exponential equation of the form:

$$r = kP_H^a P_U^b P_S^c$$

This equation is simpler to use than the more complicated L-H equations. The argument is that if it is not possible to discriminate between the various theoretical mechanisms, one might just as well use a simplified equation for design work. This would be a valid approach provided that the simplified equation provided as good a fit as the best mechanistic equation. The same data on codimer hydrogenation was fitted.

DATA TREATMENT

Table 1 lists the experimental data used in this study. The data covers three temperature levels - 200°C, 275°C and 325°C. The partial pressures of the components and the temperatures are average values over the length of the reactor. For each of the three temperatures, the data were analyzed by a linear and a non-linear regression program.

Linear Regression

A linear least squares regression computer program was used. The three kinetic equations were linearized as follows:

Mechanism (d) - molecularly adsorbed hydrogen

$$r = \frac{E_k K_H K_U P_H P_U}{(1 + K_H P_H + K_U P_U + K_S P_S)^2}$$

$$R = \sqrt{\frac{P_H P_U}{r}} = \sqrt{\frac{1}{E_k K_H K_U}} (1 + K_H P_H + K_U P_U + K_S P_S) = a + b P_H + c P_U + d P_S$$

Finally,

$$\sqrt{\frac{P_H P_U}{r}} = a + b P_H + c P_U + d P_S$$

where,

$$K_H = \frac{b}{a}$$

$$K_U = \frac{c}{a}$$

$$K_S = \frac{d}{a}$$

$$E_k = \frac{1}{a^2 K_H K_U}$$

Mechanism (h) - atomically adsorbed hydrogen

$$r = \frac{E_k K_H K_U P_H P_U}{(1 + \sqrt{K_H P_H} + K_U P_U + K_S P_S)^3}$$

$$R = \sqrt[3]{\frac{P_H P_U}{r}} = \frac{1}{E_k K_H K_U} (1 + \sqrt{K_H P_H} + K_U P_U + K_S P_S) = a + b\sqrt{P_H} + cP_U + dP_S$$

Finally,

$$\sqrt[3]{\frac{P_H P_U}{r}} = a + b\sqrt{P_H} + cP_U + dP_S$$

where,

$$K_H = \left(\frac{b}{a}\right)^2$$

$$K_U = \frac{c}{a}$$

$$K_S = \frac{d}{a}$$

$$E_k = \frac{1}{a^3 K_H K_U}$$

The development of these equations was shown by Hougen and Watson (5).

Exponential Equation

$$r = k P_H^a P_U^b P_S^c$$

$$\ln(r) = \ln(k) + a \ln(P_H) + b \ln(P_U) + c \ln(P_S)$$

After the values of the linear parameters a, b, c, and d were obtained, they were converted to the fundamental constants K_H , K_U , K_S , and E_k . The computer print-out sheets for all the linear regression runs are assembled in the Appendix.

Non-Linear Regression

A non-linear least squares computer program was used. This program uses the Marquardt method of search for the parameter values that

give a minimum for the sum of residual squares. The user must supply the partial derivative of the dependent variable, in this case the reaction rate r , with respect to each of the parameters. The partial derivatives for each equation are given in Table A in the Appendix.

The ability of the method to converge depends greatly on the initial parameter estimates supplied by the user. In all the cases the parameter results from linear regression were used as the initial estimates for the non-linear regression. In some cases the regression was also run with initial parameters which were 10% higher and 10% lower than the parameters from linear regression. The computer print-out sheets for all the non-linear regression runs are in the Appendix.

Error Calculation

For each of the three equations a Fortran program was written to calculate the residual error. After finding the values of the parameters by linear and non-linear regression, these values were used in the error program to calculate the percent error for each data point $[(r_{exp} - r_{calc})/r_{calc}]$. The average error for all the data points was also calculated, as well as the sum of the residual squares (ϕ). A listing of the computer programs used to calculate the residual error is in the Appendix.

DISCUSSION OF RESULTS

An attempt was made to estimate the degree of experimental error in the data. Table 2 tabulates the eight duplicate runs that were made. There were not enough duplicate runs made to establish a firm level of experimental error. The average percent error shown in Table 2 is $\pm 8\%$. This is certainly an indication of the order of magnitude of the experimental error. For each duplicate set of two points, the variance is calculated according to the following formula:

$$s^2 = \frac{\sum_1^n (r - \hat{r})^2}{n-1} = \frac{2(r - \hat{r})^2}{1}$$

Figure 1 is a plot of the variance for each of the duplicate points versus the average value. It suggests that the errors tend to be larger at higher values of the reaction rate. This is consistent with many situations, where the percent error is fairly constant, but the absolute error is not.

Least squares theory is based on a variance that is constant throughout the range of data. These data do not possess that property. Consequently, least squares regression does not represent a rigorous solution for the best fit. A weighted least squares regression would be indicated to find the best fit.

Table 3 gives the results of both linear and non-linear fitting of the experimental data with mechanism (d). The overall average error

for the three temperature sets is 16.9% with linear regression. The total sums of residual squares for all forty data points is 202×10^{-6} . With non-linear regression, the values of the parameters were somewhat different. However, the fit was not significantly better. The total sum of residual squares was slightly lower at 180×10^{-6} . The average percent residual error, on the other hand, was slightly larger at $\pm 18.2\%$ versus 16.9% with linear regression. In view of the lack of certainty about the variance of the experimental error, one is not justified in claiming much improvement of fit between 202×10^{-6} and 180×10^{-6} sum of residual squares.

Table 4 shows the linear and non-linear fitting of the experimental data with mechanism (h). The results show the same trends as with mechanism (d). The total sum of residual squares is 215×10^{-6} with linear regression and 189×10^{-6} with non-linear regression. The average percent error, on the other hand, showed no improvement.

For both mechanisms and regression methods, the average percent error of $\pm 17\%$ is significantly higher than the estimated experimental error of about $\pm 8\%$ between duplicates (Table 2). This does not necessarily represent lack of fit. At least part of this higher percent error arises because the experimental error does not have a constant variance. In the regression program, after the sum of residual squares has been minimized, the data points with the lowest absolute value of

the reaction rate will sometimes show an abnormally high percent error. These few very high percent errors raise the overall percent error substantially. This can be seen in the computer print-out sheets from the error calculation program (pages 49, 50, 51, 88, 89, 90, 124, 125, 126, 137, 138 and 139 in Appendix).

In comparing the results in Tables 3 and 4, it can be seen that with linear regression it is not possible to discriminate between mechanisms (d) and (h). This is in disagreement with Tschernitz, et al. They reported that the error was 17% for mechanism (d) and 34% for mechanism (h). On this basis they selected mechanism (d) as the acceptable mechanism. The present results are more in agreement with Blakemore and Hoerl. There is no way of knowing why Tschernitz, et al found the higher error with mechanism (h). However, since computers were not available at that time, the 34% error could represent a computational error in hand calculation.

Another conclusion evident from Tables 3 and 4 is that non-linear regression is not any better able than linear regression to discriminate between the two plausible mechanisms. This does not really contradict the findings of other workers who found slight to major improvement in the data fit with non-linear regression compared to linear regression. In this work, there was a slight reduction in the sum of residual squares with non-linear fitting. However, it was not sufficient to allow choosing between the two plausible mechanisms. The more meaningful average percent error did not improve with non-linear regression.

Even though the deviation is approximately the same for both mechanisms, it is instructive to make a further comparison of the fit of the two equations. One such check is a plot of the residuals versus the predicted values of the dependent variable. In Figures 2 to 4, the difference between the experimental and the predicted reaction rate is plotted against the predicted reaction rate for mechanism (d). This is shown for each temperature set. The residuals appear randomly distributed above and below the x-axis as one goes from low to high value of reaction rate. There is no trend to suggest the fit is inadequate. Figures 5 to 7 show the same plots for mechanism (h). Again, there is no reason to conclude on the basis of these plots that the fit is not acceptable.

Linear regression was applied to synthetic data generated from known parameters. One purpose was to ensure that the regression technique and the mechanics used were sound. Another purpose was to determine if there is any extraneous error introduced due to the use of the linearized form of the equation. The values of the parameters found for mechanism (d) by linear regression in Table 3 were selected as the known parameters. These constants were used together with the experimental values of the independent variables P_H , P_U , and P_S to generate a set of synthetic data for both mechanisms, which is listed in Table 5.

The synthetic data for both mechanisms was subjected to linear regression. Table 6 shows the results. The constants found were exactly the same as the known constants used to generate the data. These results show that the computer program and computational techniques were sound. They also indicate that there is no extraneous error factor introduced in using the linearized form of these two particular equations.

Another area of investigation was the use of synthetic data with error added. To the synthetic reaction rates in Table 5 was added an average error of 15%. The individual errors ranged from 3 to 45%, to agree with the general range of residual error found by regression. The error was assigned randomly. Table B in the Appendix is a listing showing how the error was introduced. Table 7 gives the synthetic data with the 15% error added.

The results for mechanism (d) are given in Table 8. Linear regression was able to establish values of the parameters to give a residual error approximately equal to the 15% error introduced. In fact, the error was slightly less. The value of the parameters found were not the same as those used to generate the data. Non-linear regression could do nothing further, as shown in Table 8. The results for mechanism (h) in Table 9 show the same findings as for mechanism (d).

The question arises whether or not there is any possibility of distinguishing between the two plausible mechanisms with the given data. To explore this question, the synthetic data with no error generated from the equation for mechanism (d) was fitted to the equation for mechanism (h) by linear regression. Table 10 shows that the constants obtained were quite different from the known constants used to generate the synthetic data. However, the total sum of residual squares was only 8×10^{-6} for all three temperature sets, comprising 40 data points. The average error was only 2.8%. This analysis indicates that if mechanism (d) were the true mechanism, one could be led into accepting mechanism (h) as a possible mechanism. The conclusion that can be drawn is that with the range of data available, discrimination between the two mechanisms is not possible. The experimental error would obscure any difference in fit of the two equations. This conclusion agrees with that of Blakemore and Hoerl, although they did not use the synthetic data technique.

The second objective of this study was to compare the use of the non-theoretical, exponential form of equation to represent the data. The equation under study was given on page 4. The results of fitting the experimental data to this equation are given in Table 11. With linear regression, the total sum of residual squares for all 40 data points was 460×10^{-6} , which is somewhat

greater than with the two theoretical equations. This is particularly true for the data set at 275 C. Non-linear regression reduced the residual sum of squares to 317×10^{-6} . Although this is slightly higher than for the two theoretical equations, it is noted that the more meaningful average percent error at $\pm 17\%$ is the same as with the theoretical equations.

The above results would seem to confirm the suggestion of Weller that for engineering work the simpler equation can be as adequate as the more complicated theoretical models. Weller used an equation of the following form:

$$r = k \cdot P_H^{1/2} \cdot P_U^{1/2}$$

There does not seem to be any real justification for limiting the equation to simple powers; such as, 0, 0.5, 1.0, as recommended by Weller. It also does not seem justified to eliminate the P_S term, as done by Weller, just because the dependence of the reaction rate on P_S is small. The average percent error of $\pm 17\%$ found for the exponential form of equation was lower than found by Weller using the above equation. He found an overall deviation of $\pm 24\%$ for the three temperature sets.

CONCLUSION

Non-linear least squares regression provided no better fit for the experimental data than the linear least squares regression. This conclusion applies to the mechanisms studied and the particular data used. It would not necessarily apply to all gas phase catalytic reactions.

With regression of the experimental data, one cannot discriminate between mechanisms (d) and (h). Both fit the data equally well.

Using synthetic data with a known amount of error, it was found that linear regression and non-linear regression (with initial values of the parameters obtained from linear regression) could fit the data without introducing any extraneous error. Because of the difficulty in obtaining initial values of the parameters which will allow convergence to the best fit, an attempt to use non-linear regression by itself could lead to extraneous error. In this study, when using non-linear regression, the initial parameters were always obtained from prior linear fitting.

In the general case of kinetic modeling of gas-phase reactions, it is concluded that for the initial screening of all the possible mechanisms, linear regression would be quite satisfactory. For discriminating between plausible mechanisms, as found by linear regression, it would be worthwhile to employ non-linear regression. However,

the present study indicates that it will give no assurance of any better fit.

A non-catalytic exponential form of equation was found to provide as satisfactory a fit with the experimental data as the two theoretical Langmuir-Hinshelwood equations.

RECOMMENDATIONS

An area for further study would be a weighted least squares regression of the experimental data used in this study. This could probably produce values of the parameters which would reduce the average percent deviation somewhat. It is very doubtful, however, if it could discriminate between the two plausible mechanisms.

A major, but informative, study would be to collect data at higher pressures and attempt to discriminate between the two mechanisms.

GLOSSARY

- r = Reaction rate, lb mols/hr · lb catalyst
- P_H = Average partial pressure of hydrogen, atm.
- P_U = Average partial pressure of unsaturate, atm.
- P_S = Average partial pressure of saturate, atm.
- E_k = Reaction rate constant and effectiveness factor,
lb mols/hr lb·catalyst
- K_H = Adsorption constant for hydrogen, atm.⁻¹
- K_U = Adsorption constant for unsaturate, atm.⁻¹
- K_S = Adsorption constant for saturate, atm.⁻¹
- ϕ = Sum of residual squares

REFERENCES

1. Bard, Y., and L. Lapidus, Catalyst Reviews, 2(1), 67 (1968).
2. Blakemore, J., and A. Hoerl, CEP Symposium Series, 42, 59, 14 (1963).
3. Chou, C., I & EC, 50, 799 (1958).
4. Draper, ., and . Smith, "Applied Regression Analysis", Wiley (1966).
5. Hougen, O., and C. Watson, "Chemical Process Principles, Vol. III, Wiley (1947).
6. Hunter, W., and J. Kittrell, "Statistical Methodology for Chemical Reaction Modelling", AICHE Today Series, February 18-19, 1967.
7. Kittrell, J., W. Hunter, and C. Watson, AICHE Journal, 11, 1051 (1965).
8. Kittrell, J., R. Mezaki, and C. Watson, I & EC, 57, 19 (1965).
9. Lapidus, L., and T. Peterson, AICHE Journal, 11, 891 (1965).
10. Tschernitz, J., S. Bornstein, R. Beckmann, and O. Hougen, Trans. Am. Inst. Chem. Engrs., 41, 445 (1945).
11. Weller, S., AICHE Journal, 2, 59 (1956).
12. Yang, K., and O. Hougen, CEP, 46, 146 (1950).

TABLE 1

Experimental Data¹

Reactor Temperature - 200°C

Data Point	Run	π (atm)	pH (atm)	p_U (atm)	p_S (atm)	$r\left(\frac{\text{lb} - \text{mol}}{(\text{lb})(\text{hr})}\right)$
1	1d	1.09	0.482	0.100	0.508	0.00353
2	3c	3.50	2.459	0.527	0.515	0.0250
3	3d	3.49	2.450	0.530	0.515	0.0320
4	10a	3.51	0.477	0.494	2.538	0.00553
5	11a	1.51	0.514	0.540	0.455	0.00870
6	11d	1.50	0.473	0.552	0.473	0.01392
7	11e	1.50	0.470	0.558	0.473	0.00960
8	12ab	1.105	0.104	0.562	0.440	0.00514
9	14a	3.52	0.450	2.840	0.230	0.01920
10	14b	3.51	0.409	2.810	0.289	0.0206
11	25a	2.50	0.484	1.075	0.942	0.0131
12	28a	2.10	0.357	1.590	0.153	0.0186

Reactor Temperature - 275°C

1	2a	1.105	0.478	0.102	0.525	0.00298
2	4d	3.520	2.505	0.518	0.497	0.0389
3	4e	3.500	2.500	0.517	0.485	0.0450
4	5b	3.510	0.425	2.770	0.310	0.0206
5	5d	3.500	0.433	2.800	0.270	0.0185
6	6bc	1.104	0.489	0.562	0.051	0.0180
7	7b	1.500	0.546	0.506	0.446	0.0103
8	7cd	1.500	0.469	0.556	0.475	0.01215
9	8bc	1.109	0.100	0.540	0.464	0.00705
10	9a	3.500	0.422	0.462	2.615	0.00824
11	9b	3.510	0.467	0.485	2.555	0.00734
12	26ab	2.500	1.495	0.511	0.495	0.0319
13	29ab	2.100	1.222	0.776	0.103	0.0435

¹ Data collected by Tschernitz, et al (Reference 10).
See also Hougen and Watson (Reference 5).

TABLE 1 (continued)

Experimental Data

Reactor Temperature - 325°C

<u>Data Point</u>	<u>Run</u>	<u>π (atm)</u>	<u>pH (atm)</u>	<u>p_U (atm)</u>	<u>p_S (atm)</u>	<u>$r \left(\frac{\text{lb - mol}}{(\text{lb})(\text{hr})} \right)$</u>
1	15a	3.50	0.500	2.735	0.270	0.0201
2	16a	1.10	0.482	0.560	0.062	0.0114
3	17b	1.50	0.501	0.533	0.466	0.0134
4	17c	1.50	0.475	0.553	0.471	0.00946
5	17e	1.50	0.476	0.556	0.478	0.00871
6	18a	1.10	0.101	0.548	0.451	0.0025
7	19b	3.50	2.335	0.550	0.610	0.0338
8	19c	3.50	2.540	0.452	0.510	0.0286
9	19d	3.50	2.405	0.524	0.572	0.0297
10	20ab	1.10	0.489	0.098	0.513	0.0044
11	21a	3.51	0.480	0.480	2.550	0.01106
12	24a	2.50	0.555	0.299	1.645	0.00533
13	27a	2.50	0.599	0.996	0.907	0.01885
14	30a	2.10	0.438	1.523	0.136	0.01414
15	30b	2.10	0.478	1.480	0.144	0.0159

TABLE 2

Error with Duplicate Sets of Data
(Data from TABLE 1)

<u>200°C</u>	<u>P_H</u>	<u>P_U</u>	<u>P_S</u>	<u>r</u>	<u>r_i-r_{avg}</u>	Variance <u>S² x 10⁻⁶</u>	<u>(r_i-r_{avg})/r_{avg}</u>
2	2.459	0.527	0.515	0.0250			
3	2.450	0.520	0.515	0.0320			
				<u>0.0285</u> avg	0.0035	24	± 12%
6	0.473	0.552	0.473	0.01392			
7	0.470	0.558	0.473	0.00960			
				<u>0.01176</u> avg	0.00216	10	± 18%
<u>275°C</u>							
2	2.505	0.518	0.497	0.0389			
3	2.500	0.517	0.485	0.0450			
				<u>0.0420</u> avg	0.0030	18	± 7%
4	0.425	2.770	0.310	0.0206			
5	0.433	2.800	0.270	0.0185			
				<u>0.0196</u> avg	0.0011	2	± 5%
7	0.546	0.506	0.446	0.01030			
8	0.469	0.556	0.475	0.01215			
				<u>0.01122</u> avg	0.00093	2	± 8%
<u>325°C</u>							
4	0.475	0.553	0.471	0.00946			
5	0.476	0.556	0.478	0.00871			
				<u>0.00908</u> avg	0.00038	0	± 4%
14	0.438	1.523	0.136	0.01414			
15	0.478	1.480	0.144	0.0159			
				<u>0.01502</u> avg	0.00088	2	± 6%
7	2.335	0.550	0.610	0.0338			
9	2.405	0.524	0.572	0.0297			
				<u>0.0318</u> avg	0.0021	8	± 6%
							± 8% avg

TABLE 3

Results of Linear and Non-Linear Regression of Experimental Data
Mechanism (d) - Molecularly Adsorbed Hydrogen

$$r = \frac{E_k K_H K_U (P_H P_U)}{(1 + K_H P_H + K_U P_U + K_S P_S)^2}$$

	Linear Regression			Non-Linear Regression ¹		
	200°C	275°C	325°C	200°C	275°C	325°C
a	2.768	2.793	3.659			
b	1.134	0.697	0.743			
c	1.528	1.623	1.650			
d	1.016	0.530	0.065			
K _H = b/a	0.410	0.250	0.203	0.344	0.238	0.191
K _U = c/a	0.552	0.581	0.451	0.516	0.589	0.415
K _S = d/a	0.367	0.190	0.018	0.514	0.232	0.001
E _k = 1/a ² K _H K _U	0.577	0.883	0.816	0.699	0.942	0.889
<u>Error</u>						
φ	68 x 10 ⁻⁶	98 x 10 ⁻⁶	36 x 10 ⁻⁶	61 x 10 ⁻⁶	85 x 10 ⁻⁶	34 x 10 ⁻⁶
Avg(r _{exp} - r _{calc})/r _{calc}	17.0	19.5	14.1	21.4	19.2	13.9
Avg error for three temperatures	----- ±16.9 -----			----- ±18.2 -----		

NOTES:

¹ Initial estimates of parameters were those obtained by linear regression.

TABLE 4

Results of Linear and Non-Linear Regression of Experimental Data
 Mechanism (h) - Atomically Adsorbed Hydrogen

$$r = \frac{E_k K_H K_U P_H P_U}{(1 + \sqrt{K_H P_H} + K_U P_U + K_S P_S)^3}$$

	Linear Regression			Non-Linear Regression		
	200°C	275°C	325°C	200°C	275°C	325°C
a	1.652	1.728	2.166			
b	0.951	0.650	0.595			
c	0.561	0.608	0.594			
d	0.370	0.219	0.014			
$K_H = (b/a)^2$	0.331	0.141	0.075	0.263	0.128	0.075
$K_U = c/a$	0.339	0.352	0.274	0.324	0.371	0.271
$K_S = d/a$	0.224	0.127	0.006	0.197	0.178	0.009
$E_k = 1/a^3 K_H K_U$	1.977	3.905	4.788	2.297	4.336	4.788
<u>Error</u>						
ϕ	62 x 10 ⁻⁶	113 x 10 ⁻⁶	40 x 10 ⁻⁶	60 x 10 ⁻⁶	89 x 10 ⁻⁶	40 x 10 ⁻⁶
Avg($r_{exp} - r_{calc}$)/ r_{calc}	14.7	17.2	15.6	15.3	17.3	15.8
Avg error for three temperatures	----- ±15.8 -----			----- ±16.1 -----		

TABLE 5

Synthetic Data - No Error

Synthetic Reaction Rates Generated from Known Parameters
and Experimental Partial Pressures

<u>Known Parameters</u>	<u>Mechanism (d)</u>			<u>Mechanism (h)</u>		
	<u>200°C</u>	<u>275°C</u>	<u>325°C</u>	<u>200°C</u>	<u>275°C</u>	<u>325°C</u>
K _H	0.410	0.250	0.203	0.410	0.250	0.203
K _U	0.552	0.581	0.451	0.552	0.581	0.451
K _S	0.367	0.190	0.018	0.367	0.190	0.018
E _k	0.577	0.883	0.816	0.577	0.883	0.816
<u>Data Point</u>						
1	3,038 x 10 ⁻⁶	3,825 x 10 ⁻⁶	18,660 x 10 ⁻⁶	1,312 x 10 ⁻⁶	1,835 x 10 ⁻⁶	6,111 x 10 ⁻⁶
2	27,335	40,719	11,039	11,041	15,915	5,245
3	27,435	40,725	10,938	11,065	15,932	5,177
4	5,343	19,614	10,699	1,660	5,624	5,086
5	12,906	20,028	10,753	5,088	5,718	5,107
6	12,192	16,570	2,540	4,827	7,356	1,511
7	12,216	15,433	31,944	4,834	6,632	12,988
8	3,328	14,277	28,702	1,614	6,179	11,910
9	20,741	3,401	31,281	5,702	1,824	12,788
10	18,807	7,144	2,694	5,203	2,738	1,396
11	14,870	8,184	9,308	5,010	3,097	4,409
12	17,129	31,463	7,600	5,963	12,205	3,672
13		38,562	17,694		14,686	7,464
14			15,760			6,347
15			16,924			6,792
<u>Error</u>						
φ	0	0	0	0	0	0

TABLE 6

Linear Regression of Synthetic Data with No Error
Generated from Known Parameters¹

	<u>Mechanism d</u> <u>No Dissociation of H₂</u>		<u>Mechanism h</u> <u>Dissociation of H₂</u>	
	<u>Known</u> <u>Parameter</u>	<u>Results of</u> <u>Regression</u>	<u>Known</u> <u>Parameter</u>	<u>Results of</u> <u>Regression</u>
<u>200°C</u>				
K _H	0.410	0.410	0.410	0.410
K _U	0.552	0.552	0.552	0.552
K _S	0.367	0.367	0.367	0.367
E _k	0.577	0.577	0.577	0.577
Avg Error		0.0		0.0
<u>275°C</u>				
K _H	0.250	0.252	0.250	0.250
K _U	0.581	0.581	0.581	0.581
K _S	0.190	0.190	0.190	0.190
E _k	0.883	0.883	0.883	0.883
Avg Error		0.0		0.0
<u>325°C</u>				
K _H	0.203	0.203	0.203	0.203
K _U	0.451	0.451	0.451	0.451
K _S	0.018	0.018	0.018	0.018
E _k	0.816	0.816	0.816	0.816
Avg Error		0.0		0.0

NOTES

¹ Synthetic data as given in Table 5

TABLE 7

Synthetic Data - 15% Error

Synthetic Reaction Rates Generated from Known Parameters
with 15% Random Error

<u>Known Parameters</u>	<u>Mechanism (d)</u>			<u>Mechanism (h)</u>		
	<u>200°C</u>	<u>275°C</u>	<u>325°C</u>	<u>200°C</u>	<u>275°C</u>	<u>325°C</u>
K_H	0.410	0.250	0.203			
K_U	0.552	0.581	0.451			
K_S	0.367	0.190	0.018		S A M E	
E_k	0.577	0.883	0.816			
<u>Data Point</u>						
1	$2,855 \times 10^{-6}$	$5,546 \times 10^{-6}$	$18,100 \times 10^{-6}$	$1,233 \times 10^{-6}$	$2,661 \times 10^{-6}$	$5,927 \times 10^{-6}$
2	30,068	44,790	10,045	12,145	17,506	4,773
3	30,727	43,983	9,407	12,393	17,206	4,452
4	4,862	18,437	12,732	1,510	5,286	6,052
5	13,938	17,224	15,592	5,495	4,917	7,405
6	10,485	14,084	2,794	5,613	6,252	1,662
7	14,537	9,568	34,500	5,752	4,112	14,027
8	2,962	15,934	22,962	1,436	6,920	9,528
9	21,778	3,571	27,840	5,987	1,915	11,381
10	18,243	6,358	2,532	5,047	2,437	1,312
11	9,219	7,938	10,425	3,106	3,004	4,938
12	24,837	28,631	4,712	8,646	11,106	2,277
13		45,888	15,925		17,476	6,718
14			13,396			5,395
15			17,770			7,132
<u>Error</u>						
ϕ	120×10^{-6}	145×10^{-6}	101×10^{-6}	15×10^{-6}	22×10^{-6}	19×10^{-6}
Avg($r_{exp} - r_{calc}$)/ r_{calc}	15.0	14.9	15.0	15.2	14.9	15.0

TABLE 8

Linear and Non-Linear Regression of Synthetic Data
Generated from Known Parameters - with 15% Random Error Added¹

	Mechanism (d) - Molecularly Adsorbed H ₂		
	<u>Known Parameters</u>	<u>Parameters Found by Linear Regression</u>	<u>Parameters Found by Non-Linear Regression</u>
<u>200°C</u>			
K _H	0.410	0.339	0.344
K _U	0.552	0.545	0.545
K _S	0.367	0.497	0.486
E _k	0.577	0.713	0.717
φ	120 x 10 ⁻⁶	86 x 10 ⁻⁶	85 x 10 ⁻⁶
Avg % error	15.0	12.5	12.1
<u>275°C</u>			
K _H	0.250	0.201	0.206
K _U	0.581	0.638	0.640
K _S	0.190	0.210	0.216
E _k	0.883	0.987	0.991
φ	145 x 10 ⁻⁶	110 x 10 ⁻⁶	107 x 10 ⁻⁶
Avg % error	14.9	13.2	12.6
<u>325°C</u>			
K _H	0.203	0.251	0.256
K _U	0.451	0.479	0.492
K _S	0.018	0.048	0.071
E _k	0.816	0.659	0.666
φ	101 x 10 ⁻⁶	89 x 10 ⁻⁶	88 x 10 ⁻⁶
Avg % error	15.0	14.6	15.0

NOTES

¹ Data in Table 7.

TABLE 9

Linear and Non-Linear Regression of Synthetic Data
Generated from Known Parameters - with 15% Random Error Added

	Mechanism (h) - Atomically Adsorbed H ₂		
	<u>Known Parameter</u>	<u>Parameter Found by Linear Regression</u>	<u>Parameters Found by Non-Linear Regression</u>
<u>200°C</u>			
K _H	0.410	0.333	0.343
K _U	0.552	0.576	0.571
K _S	0.367	0.490	0.470
E _k	0.577	0.736	0.745
φ	15 x 10 ⁻⁶	9 x 10 ⁻⁶	9 x 10 ⁻⁶
Avg % error	15.2	12.2	11.6
<u>275°C</u>			
K _H	0.250	0.187	0.188
K _U	0.581	0.617	0.618
K _S	0.190	0.205	0.202
E _k	0.883	1.051	1.055
φ	22 x 10 ⁻⁶	18 x 10 ⁻⁶	18 x 10 ⁻⁶
Avg % error	14.9	13.3	12.9
<u>325°C</u>			
K _H	0.203	0.302	0.306
K _U	0.451	0.488	0.500
K _S	0.018	0.041	0.056
E _k	0.816	0.599	0.604
φ	19 x 10 ⁻⁶	17 x 10 ⁻⁶	17 x 10 ⁻⁶
Avg % error	15.0	14.4	14.7

TABLE 10

Results of Fitting Synthetic Data Generated by
Mechanism (d) to Equation for Mechanism (h)

	Known Parameters Used to Generate Synthetic Reaction Rates ¹ for Mechanism (d)	Parameter Found by Regression in Fit- ting Synthetic Data ¹ to Mechanism (h)	Error Obtained With Mechanism (h) When Using Synthetic Data Generated by Mechanism (d)	
			Percent	ϕ
<u>200°C</u>				
K _H	0.410	0.254	3.4	1 x 10 ⁻⁶
K _J	0.552	0.312		
K _S	0.367	0.204		
E _k	0.577	2.371		
<u>275°C</u>				
K _H	0.250	0.098	2.72	6 x 10 ⁻⁶
K _J	0.581	0.330		
K _S	0.190	0.114		
E _k	0.883	5.146		
<u>325°C</u>				
K _H	0.203	0.073	2.3	1 x 10 ⁻⁶
K _J	0.451	0.267		
K _S	0.018	0.005		
E _k	0.816	4.896		
			2.8 avg	8 x 10 ⁻⁶

NOTES

- ¹ Synthetic reaction rates used were those under mechanism (d) in Table 5.

TABLE 11

Results of Linear and Non-Linear Regression
of Experimental Data

Mechanism - Non-Catalytic, Exponential

$$r = kP_H^a P_U^b P_S^c$$

	Linear Regression			Non-Linear Regression		
	<u>200°C</u>	<u>275°C</u>	<u>325°C</u>	<u>200°C</u>	<u>275°C</u>	<u>325°C</u>
k	0.0172	0.023	0.022	0.0182	0.0255	0.0219
a	0.597	0.704	0.771	0.569	0.735	0.732
b	0.469	0.483	0.494	0.362	0.300	0.471
c	-0.235	-0.179	-0.021	-0.168	-0.098	-0.024
<u>Error</u>						
φ	97	299	64	70	190	57
Avg($r_{exp} - r_{calc}$)/ r_{calc}	15.7	22.7	13.4	16.9	21.5	13.1
	-----	17.3	-----	-----	17.2	-----

FIGURE 1

Error for Duplicate sets of Data
Variance Versus average for Duplicates

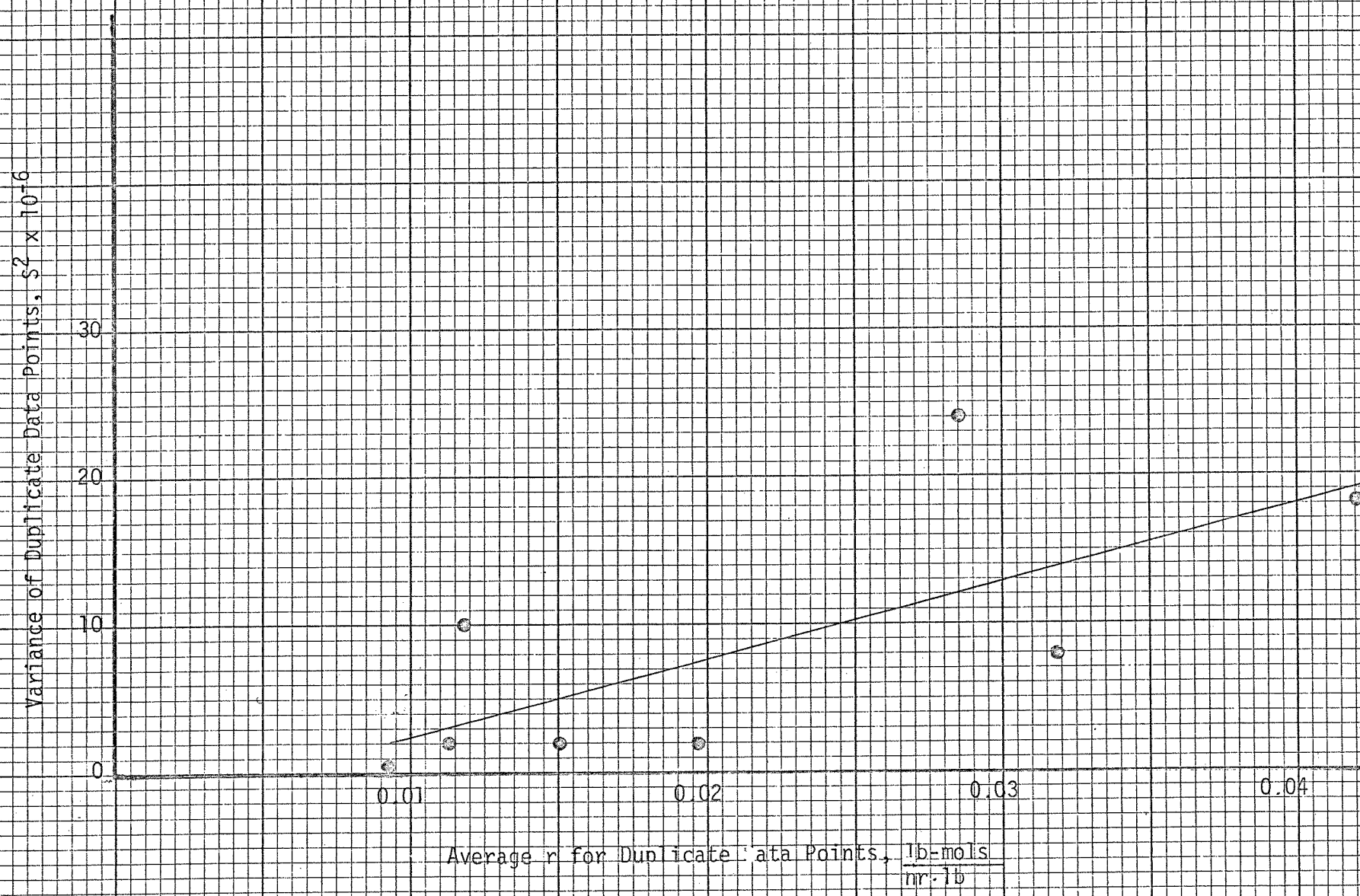


FIGURE 2
Residuals versus Predicted Reaction Rates
Mechanism (d) - Non-Linear Regression
200°C

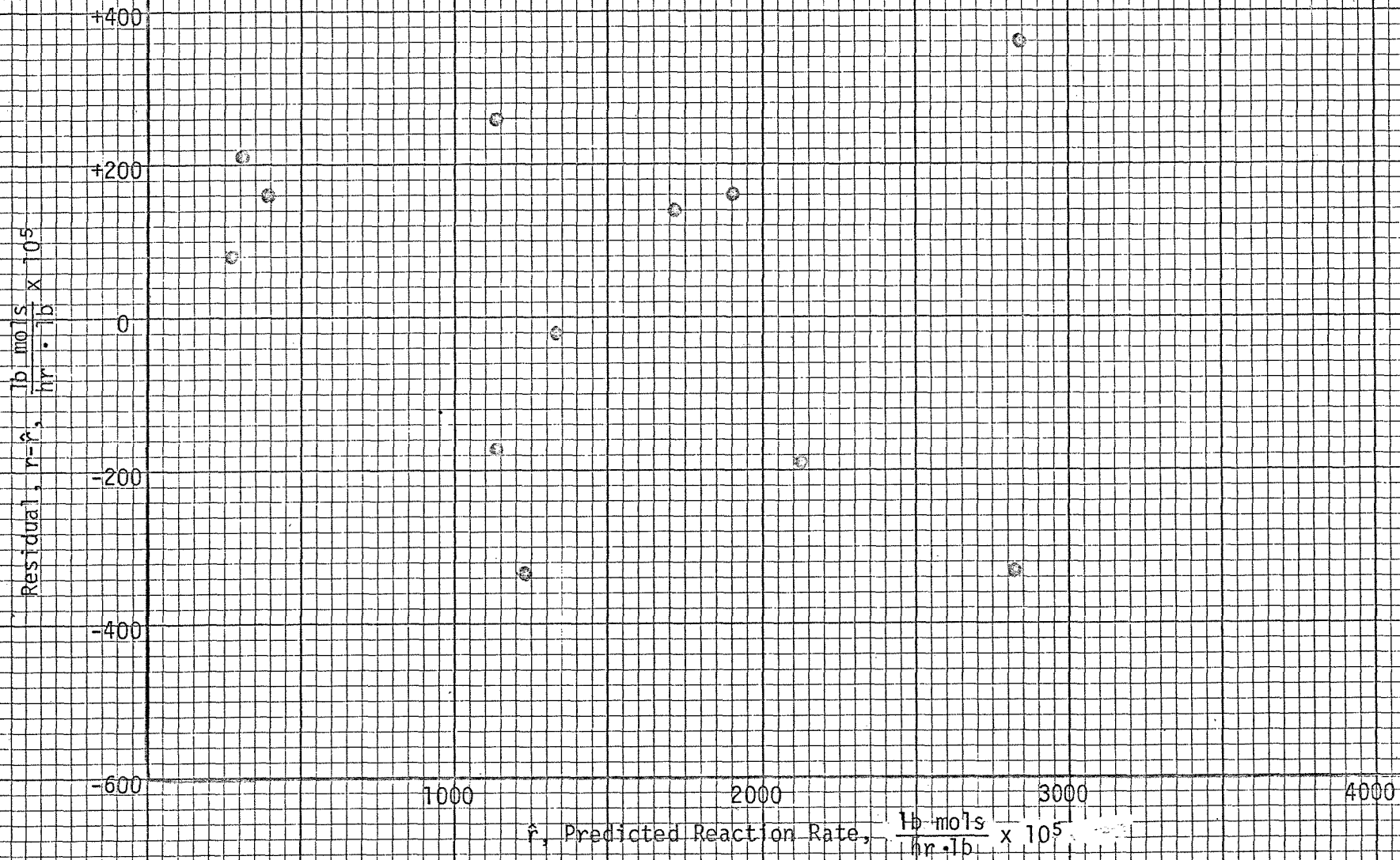


FIGURE 3
Residuals Versus Predicted Reaction Rates
Mechanism (d) - Non-Linear Regression
275°C

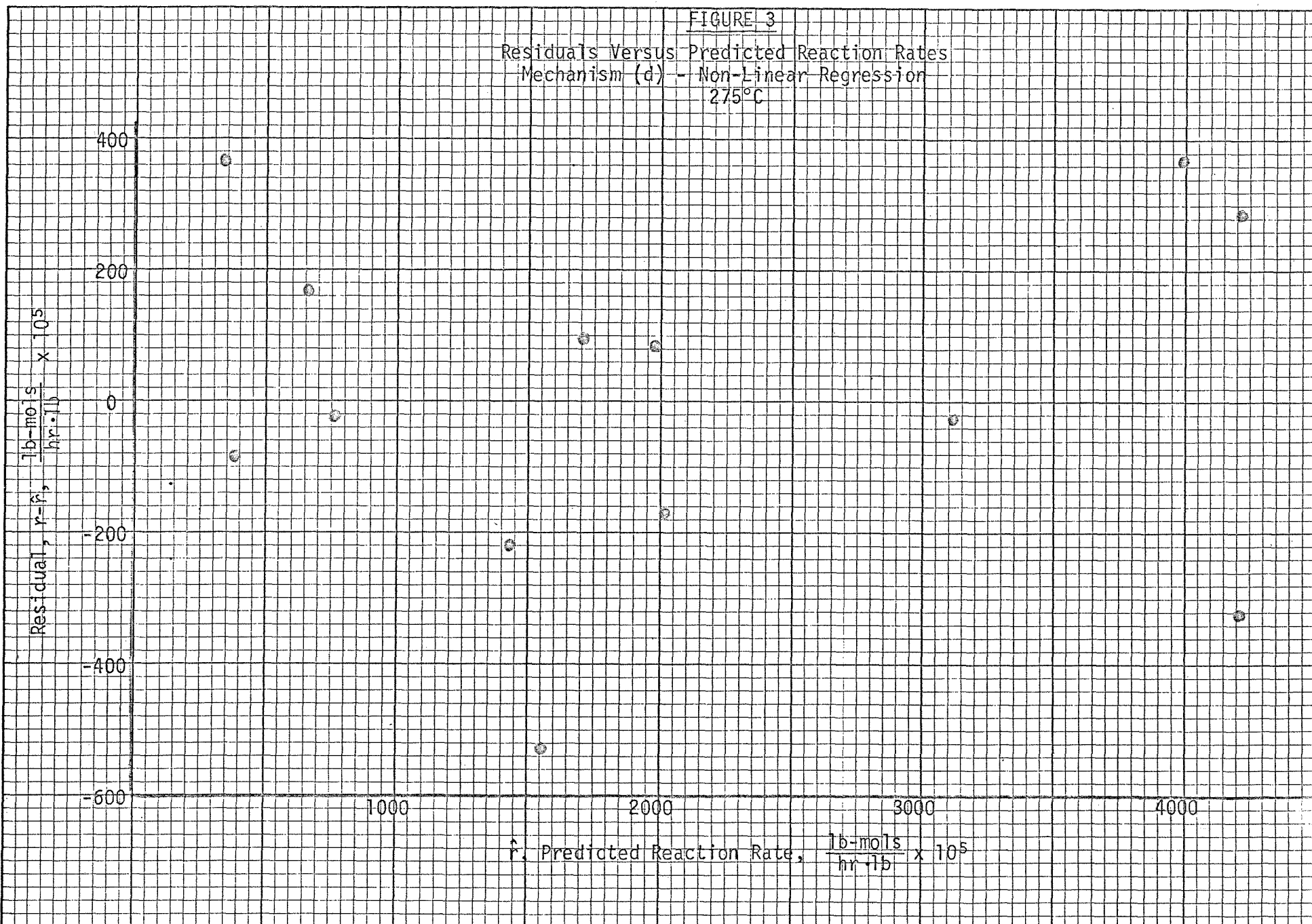


FIGURE 4

Residuals Versus Predicted Reaction Rates
Mechanism (d) - Non-Linear Regression
325°C

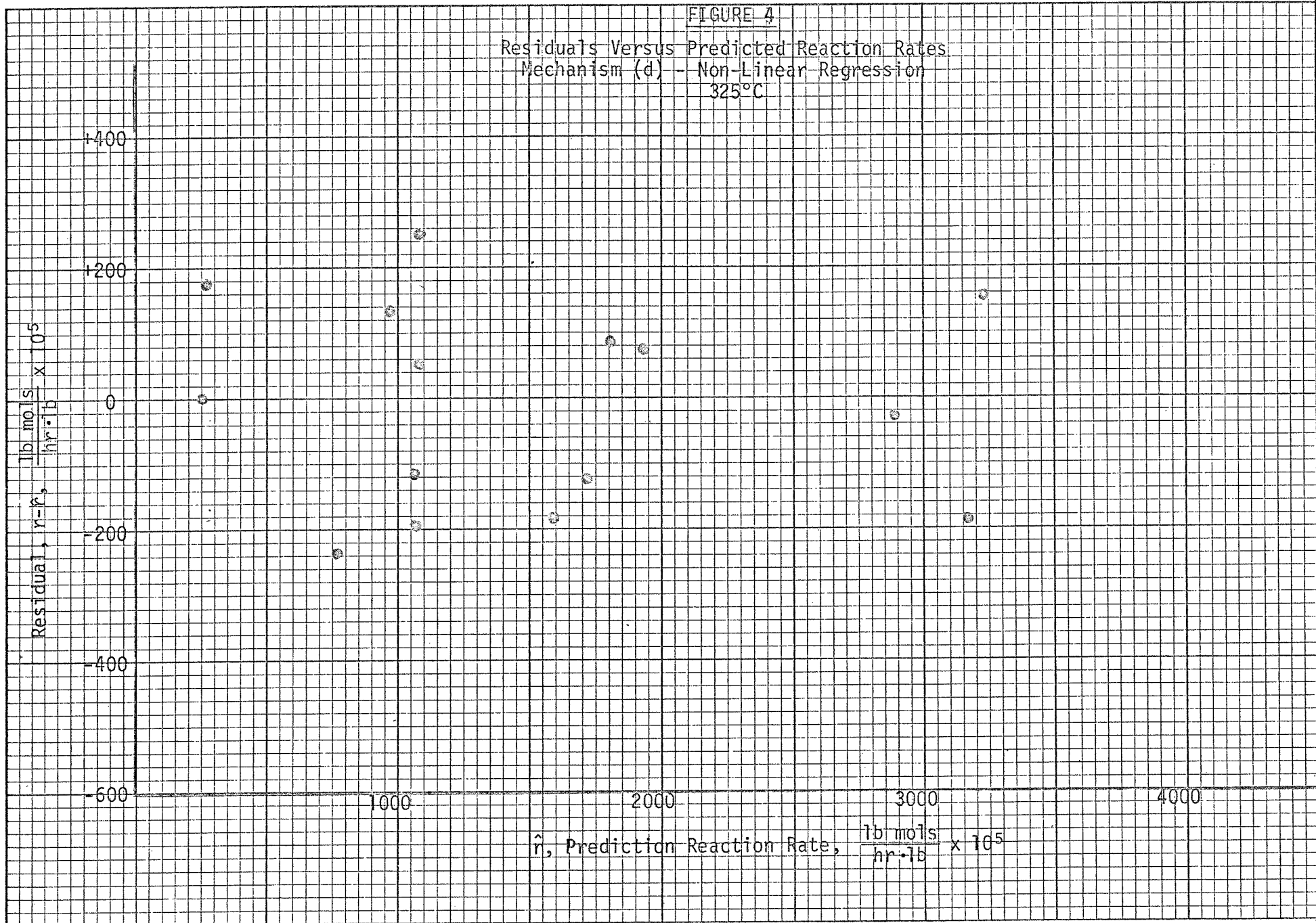


FIGURE 5

Residuals Versus Predicted Reaction Rates
Mechanism (h) - Non-Linear Regression
200°C

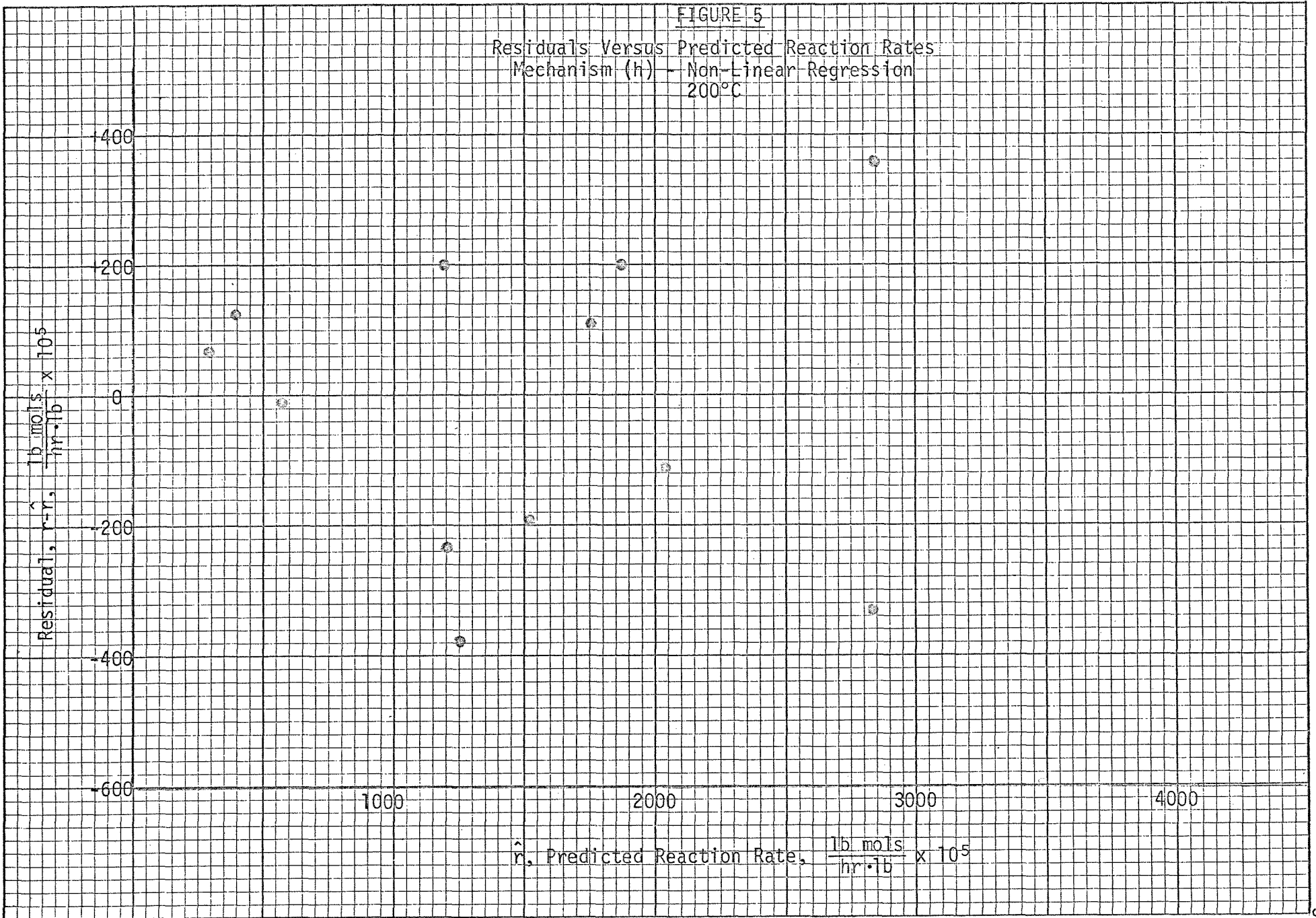


FIGURE 6
Residuals Versus Predicted Reaction Rates
Mechanism (h) - Non-Linear Regression
275°C

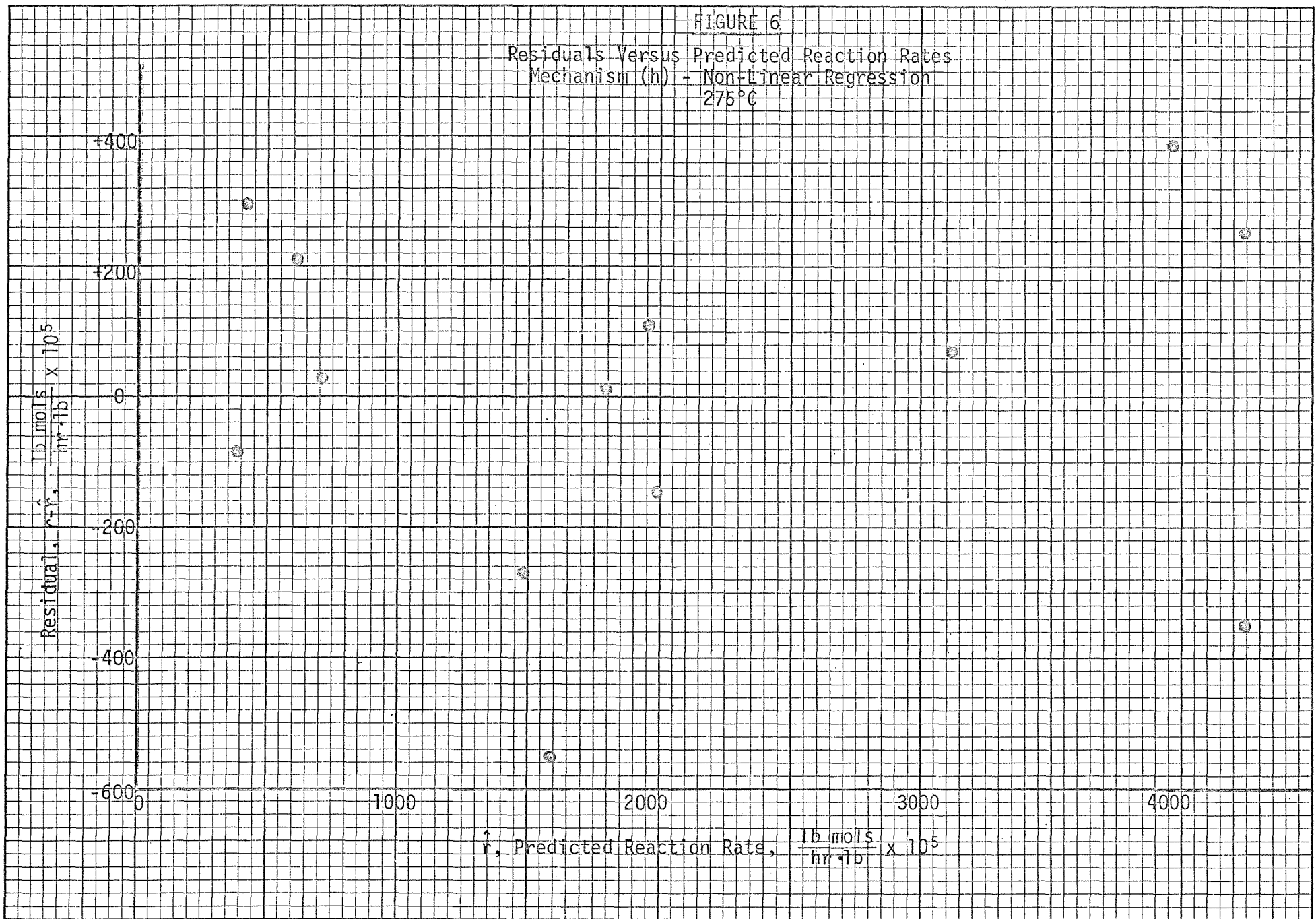
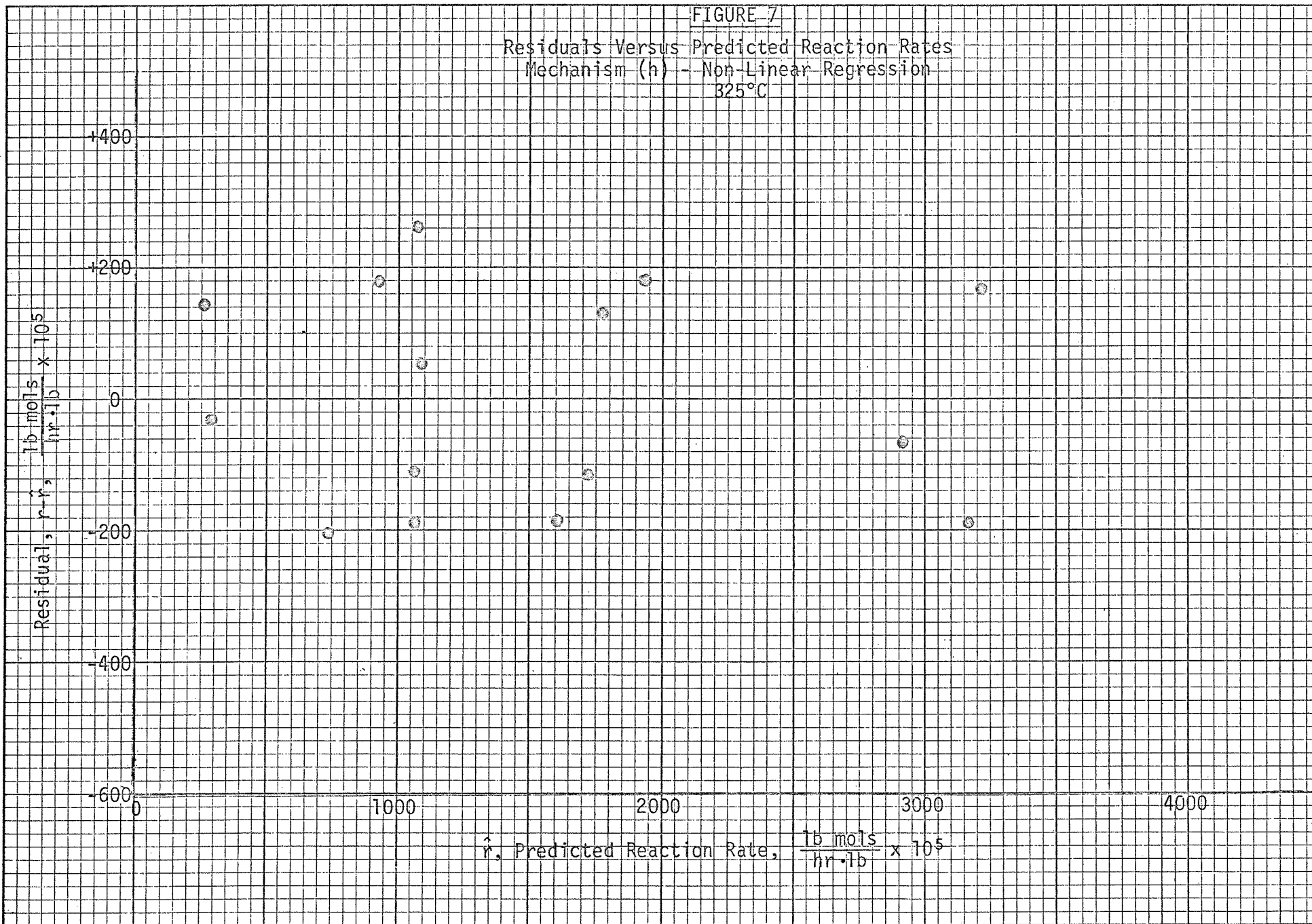


FIGURE 7

Residuals Versus Predicted Reaction Rates
Mechanism (h) - Non-Linear Regression
325°C



APPENDIX

TABLE A

Partial Derivatives Used for Non-Linear Regression Program

Mechanism (d) - molecularly adsorbed hydrogen

$$r = \frac{E_k K_H K_U P_H P_U}{(1 + K_H P_H + K_U P_U + K_S P_S)^2}$$

$$\frac{2r}{\partial K_H} = - \frac{2E_k P_H^2 P_U}{(1 + K_H P_H + K_U P_U + K_S P_S)^3}$$

$$\frac{2r}{\partial K_U} = - \frac{2E_k P_U^2 P_H}{(1 + K_H P_H + K_U P_U + K_S P_S)^3}$$

$$\frac{2r}{\partial K_S} = - \frac{2E_k P_H P_U P_S}{(1 + K_H P_H + K_U P_U + K_S P_S)^3}$$

$$\frac{2r}{\partial E_k} = \frac{P_H P_U}{(1 + K_H P_H + K_U P_U + K_S P_S)^2}$$

Mechanism (h) - atomically adsorbed hydrogen

$$r = \frac{E_k K_H K_U P_H P_U}{(1 + \sqrt{K_H P_H} + K_U P_U + K_S P_S)^3}$$

$$\frac{2r}{\partial K_H} = \frac{-1.5 E_k P_H^{1.5} P_U K_H^{0.5}}{(1 + \sqrt{K_H P_H} + K_U P_U + K_S P_S)^4}$$

$$\frac{2r}{\partial K_U} = \frac{-3 E_k P_H P_U P_S}{(1 + \sqrt{K_H P_H} + K_U P_U + K_S P_S)^4}$$

$$\frac{2r}{\partial K_S} = \frac{-3 E_k P_H P_U P_S}{(1 + \sqrt{K_H P_H} + K_U P_U + K_S P_S)^4}$$

$$\frac{2r}{\partial E_k} = \frac{P_H P_U}{(1 + \sqrt{K_H P_H} + K_U P_U + K_S P_S)^3}$$

TABLE A (continued)

Partial Derivatives Used for Non-Linear Regression Program

Exponential form of equation

$$r = k p_H^a p_U^b p_S^c$$

$$\frac{r}{\partial k} = p_H^a p_U^b p_S^c$$

$$\frac{r}{\partial a} = k p_H^a p_U^b p_S^c \ln a$$

$$\frac{r}{\partial b} = k p_H^a p_U^b p_S^c \ln b$$

$$\frac{r}{\partial c} = k p_H^a p_U^b p_S^c \ln c$$

TABLE B

Random Error Distribution¹

<u>Error on rexp</u>	<u>200°C</u> <u>Assign to Run No.</u>	<u>275°C</u> <u>Assign to Run No.</u>	<u>325°C</u> <u>Assign to Run No.</u>
- 3	10	11	1
- 5	9	9	15
- 6	1	4	10
- 8	5	3	7
- 9	4	12	2
10	2	2	13
-11	8	10	9
12	3	8	11
-14	6	5	3
19	7	13	4
-38	11	7	12
45	12	1	5
-15		6	14
10			6
-20			8

NOTES

- ¹ This table was used to introduce random errors to the synthetic reaction rates generated from known parameters given in Table 4.

TABLE C

Synthetic Reaction Rates With
15% Random Error Added

Mechanism (d): No Dissociation of H₂

	200°C			275°C			325°C		
K _H	0.410			0.250			0.203		
K _U	0.552			0.581			0.451		
K _S	0.367			0.190			0.018		
E _k	0.577			0.883			0.816		
Data Point	Synthetic Value of r	% Error	New Value of r	Synthetic Value of r	% Error	New Value of r	Synthetic Value of r	% Error	New Value of r
1	3,038 x 10 ⁻⁶	- 6	2,855 x 10 ⁻⁶	3,825 x 10 ⁻⁶	45	3,546 x 10 ⁻⁶	18,660 x 10 ⁻⁶	- 3	18,100 x 10 ⁻⁶
2	27,335	10	30,068	40,719	10	44,790	11,039	- 9	10,045
3	27,435	12	30,727	40,725	8	43,983	10,938	-14	9,407
4	5,343	- 9	4,862	19,614	- 6	18,437	10,699	19	12,732
5	12,906	8	13,938	20,028	-14	17,224	10,753	45	15,592
6	12,192	-14	10,485	16,570	-15	14,084	2,540	10	2,794
7	12,216	19	14,537	15,433	-38	9,568	31,944	8	34,500
8	3,328	-11	2,962	14,277	12	15,934	28,702	-20	22,962
9	20,741	5	21,778	3,401	5	3,571	31,281	-11	27,840
10	18,807	- 3	18,243	7,144	-11	6,358	2,694	- 6	2,532
11	14,870	-38	9,219	8,184	- 3	7,938	9,308	12	10,425
12	17,129	45	24,837	31,463	- 9	28,631	7,600	-38	4,712
13				38,562	19	45,888	17,694	-10	15,925
14							15,760	-15	13,396
15							16,924	5	17,770

TABLE C (continued)

Synthetic Reaction Rates With
15% Random Error Added

Mechanism (h): Dissociation of H₂

	200°C			275°C			325°C		
K _H	0.410			0.250			0.203		
K _T	0.552			0.581			0.451		
K _S	0.367			0.190			0.018		
E _k	0.577			0.883			0.816		
Data Point	Synthetic Value of r	% Error	New Value of r	Synthetic Value of r	% Error	New Value of r	Synthetic Value of r	% Error	New Value of r
1	1,312 x 10 ⁻⁶	- 6	1,233 x 10 ⁻⁶	1,835 x 10 ⁻⁶	45	2,661 x 10 ⁻⁶	6,111 x 10 ⁻⁶	- 3	5,927 x 10 ⁻⁶
2	11,041	10	12,145	15,915	10	17,506	5,245	- 9	4,773
3	11,065	12	12,393	15,932	8	17,206	5,177	-14	4,452
4	1,660	- 9	1,510	5,624	- 6	5,286	5,086	19	6,052
5	5,088	8	5,495	5,718	-14	4,917	5,107	45	7,405
6	4,827	-14	5,613	7,356	-15	6,252	1,511	10	1,662
7	4,834	19	5,752	6,632	-38	4,112	12,988	8	14,027
8	1,614	-11	1,436	6,179	12	6,920	11,910	-20	9,528
9	5,702	5	5,987	1,824	5	1,915	12,788	-11	11,381
10	5,203	- 3	5,047	2,738	-11	2,437	1,396	- 6	1,312
11	5,010	-38	3,106	3,097	- 3	3,004	4,409	12	4,938
12	5,963	45	8,646	12,205	- 9	11,106	3,672	-38	2,277
13				14,686	19	17,476	7,464	-10	6,718
14							6,347	-15	5,395
15							6,792	5	7,132

MECHANISM (d)
EXPERIMENTAL DATA

NO DISSOCIATION OF H2 - LINEAR MODEL - 200 DEG C

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.6130
STANDARD ERROR OF THE MEAN	0.1769
MULTIPLE R	0.9361
MULTIPLE RSQR	0.8763

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	1.01582575	0.31181389	0.7551	0.4320
PH2	1.13457274	0.24144992	0.8557	0.6093
PU	1.52774882	0.22083908	0.9256	0.9458

INSTANT 2.7677083

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.40629E 03	0.40629E 03	
REGRESSION	3	0.21315E 02	0.71053E 01	0.18908E 01
ERROR	8	0.30062E 01	0.37577E 00	

$$a = 2.768$$

$$b = 1.134$$

$$c = 1.528$$

$$d = 1.016$$

$$K_H = \frac{b}{a} = 0.410$$

$$K_U = \frac{c}{a} = 0.552$$

$$K_S = \frac{d}{a} = 0.367$$

$$ER = \frac{1}{a^2 K_H K_U} = 0.577$$

REGRESSION ANALYSIS

DEPENDENT VARIABLE
 RESIDUAL STANDARD DEVIATION 0.6045
 STANDARD ERROR OF THE MEAN 0.1676
 MULTIPLE R 0.9294
 MULTIPLE RSQR 0.8638

VARIABLE ENTERED PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COI
PS	0.53015577	0.22157532	0.6235	0.315
PH2	0.69730115	0.23091423	0.7094	0.394
PU	1.62261462	0.21638235	0.9284	0.993

STANT 2.7926173

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.34844E 03	0.34844E 03	
REGRESSION	3	0.20870E 02	0.69569E 01	0.1903
ERROR	9	0.32888E 01	0.36542E 00	

$$a = 2.793$$

$$b = 0.697$$

$$c = 1.623$$

$$d = 0.530$$

$$K_H = \frac{b}{a} = \frac{0.697}{2.793} = 0.250$$

$$K_U = \frac{c}{a} = \frac{1.623}{2.793} = 0.581$$

$$K_S = \frac{d}{a} = \frac{0.530}{2.793} = 0.190$$

$$R^2 = \frac{1}{a^2(K_H^2 + K_U^2)} = 0.883$$

NO DISSOCIATION OF H2 - LINEAR MODEL 325 DEG C

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.5075
STANDARD ERROR OF THE MEAN	0.1310
MULTIPLE R	0.9284
MULTIPLE RSQR	0.8620

INDEPENDENT VARIABLE ENTERED	PS
------------------------------	----

INDEPENDENT VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.06505261	0.22376301	0.0873	0.0347
PH2	0.74313068	0.17036637	0.7960	0.5033
PH	1.65012908	0.22276410	0.9126	0.9055

CONSTANT	3.6589160
----------	-----------

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.47813E 03	0.47813E 03	
REGRESSION	3	0.17707E 02	0.59025E 01	0.22909E 02
ERROR	11	0.28340E 01	0.25764E 00	

$$a = 3.659$$

$$b = 0.743$$

$$c = 1.650$$

$$d = 0.065$$

$$K_H = \frac{b}{a} = \frac{0.743}{3.659} = 0.203$$

$$K_U = \frac{c}{a} = \frac{1.650}{3.659} = 0.451$$

$$K_S = \frac{d}{a} = \frac{0.065}{3.659} = 0.018$$

$$E_k = \frac{1}{a^2 K_H K_U} = 0.816$$

PD

1 11/02/72

48.

JOB F 1001 2002 3003 4004 F 2

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - SYNT GROUP - CSRD

```
// FOR
*ONE WORD INTEGERS
*LIST ALL
*IOCS(CARD,1403 PRINTER)
C HYDROGENATION OF CODIMER
C PROGRAM TO CALC ERROR AFTER FINDING CONSTANTS
C MECHANISM - NO DISSOCIATION OF HYDROGEN
C
REAL KH,KU,KS
DIMENSION PH(20),PU(20),PS(20),REXP(20),RCALC(20),DIFF(20)
```

```
ICRD=2
LPRT=5
ERROR = 0.0
PHI=0.0
```

*** READ CONSTANTS ***

READ(ICRD,100) KH,KU,KS,EK

```
L=0
2 L=L+1
READ(ICRD,102) REXP(L),PH(L),PU(L),PS(L)
IF( PH(L) ) 60,30,20
20 DENOM = 1. + KH*PH(L) + KU*PU(L) + KS*PS(L)
RCALC(L) = EK*KH*KU*PH(L)*PU(L) / DENOM**2
DIFF(L) = ( REXP(L) - RCALC(L) ) / RCALC(L) * 100.
PHI = PHI + ( RCALC(L) - REXP(L) ) **2
GO TO 2
```

```
30 KOUNT = L-1
WRITE(LPRT,110)
WRITE(LPRT,111) KH
WRITE(LPRT,112) KU
WRITE(LPRT,113) KS
WRITE(LPRT,114) EK
WRITE(LPRT,120)
DO 50 L = 1, KOUNT
ERROR = ERROR + ABS(DIFF(L))
50 WRITE(LPRT,130) L,RCALC(L),REXP(L),PH(L),PU(L),PS(L),DIFF(L)
XNUM=KOUNT
ERROR = ERROR/XNUM
WRITE(LPRT,140) PHI, ERROR
```

```
60 CALL EXIT
```

```
100 FORMAT( 4F15.0 )
102 FORMAT( 10X,4F10.0 )
110 FORMAT( 1H1 )
111 FORMAT( 6H KH = , F6.4 )
112 FORMAT( 6H KU = , F6.4 )
113 FORMAT( 6H KS = , F6.4 )
114 FORMAT( 6H EK = , F6.4 / )
120 FORMAT( 3X,50H CALC EXPER PH PU PS
1 3X,20H RXN RATE RXN RATE ,35X,10H PCT ERROR )
130 FORMAT( 1X,12,5F10.5,F10.1 )
140 FORMAT( // 18H PHI = , F10.6
1 / 18H AVG PCT ERROR = , F10.1 )
```

```
END
VARIABLE ALLOCATIONS
PH(R )=0026-0000 PU(R )=004E-0028 PS(R )=0076-0050 REXP(R )=
KH(R )=00F0 KU(R )=00F2 KS(R )=00F4 ERROR(R )=
DENOM(R )=00FC XNUM(R )=00FE ICRD(I )=0104 LPRT(I )=
```

```
STATEMENT ALLOCATIONS
100 =0114 102 =0117 110 =011B 111 =011E 112 =0124 113 =012A
2 =01BD 20 =01DC 30 =0229 50 =0264 60 =0294
```

No Dissociation of H₂

47.

KH = 0.4100
KU = 0.5520
KS = 0.3670
EK = 0.5770

200°C

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00303	0.00353	0.48200	0.10000	0.50800	16.1
2	0.02733	0.02500	2.45900	0.52700	0.51500	-8.5
3	0.02743	0.03200	2.45000	0.53000	0.51500	16.6
4	0.00534	0.00553	0.47700	0.49400	2.53800	3.4
5	0.01290	0.00870	0.51400	0.54000	0.45500	-32.5
6	0.01219	0.01392	0.47300	0.55200	0.47300	14.1
7	0.01221	0.00960	0.47000	0.55800	0.47300	-21.4
8	0.00332	0.00514	0.10400	0.56200	0.44000	54.4
9	0.02074	0.01920	0.45000	2.84000	0.23000	-7.4
10	0.01880	0.02060	0.40900	2.81000	0.28900	9.5
11	0.01487	0.01310	0.48400	1.07500	0.94200	-11.9
12	0.01712	0.01860	0.35700	1.59000	0.15300	8.5

AVG PCT ERROR = PHI = 0.000068
17.0

Experimental Data - Results of Linear Regression
 No dissociation of H₂
 275°C

KH = 0.2500
 KU = 0.5810
 KS = 0.1900
 EK = 0.8830

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00382	0.00298	0.47800	0.10200	0.52500	-22.1
2	0.04071	0.03890	2.50500	0.51800	0.49700	-4.4
3	0.04072	0.04500	2.50000	0.51700	0.48500	10.4
4	0.01961	0.02060	0.42500	2.77000	0.31000	5.0
5	0.02002	0.01850	0.43300	2.80000	0.27000	-7.6
6	0.01657	0.01800	0.48900	0.56200	0.05100	8.6
7	0.01543	0.01030	0.54600	0.50600	0.44600	-33.2
8	0.01427	0.01215	0.46900	0.55600	0.47500	-14.8
9	0.00340	0.00705	0.10000	0.54000	0.46400	107.2
10	0.00714	0.00824	0.42200	0.46200	2.61500	15.3
11	0.00818	0.00734	0.46700	0.48500	2.55500	-10.3
12	0.03146	0.03190	1.49500	0.51100	0.49500	1.3
13	0.03856	0.04350	1.22200	0.77600	0.10300	12.8

PHI = 0.000098
 AVG PCT ERROR = 19.5

Experimental Data - Results of Linear Regression

No dissociation of H₂

325°C

51.

KH = 0.2030
 KU = 0.4510
 KS = 0.0180
 EK = 0.8160

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.01866	0.02010	0.50000	2.73500	0.27000	7.7
2	0.01103	0.01140	0.48200	0.56000	0.06200	3.2
3	0.01093	0.01340	0.50100	0.53300	0.46600	22.5
4	0.01069	0.00946	0.47500	0.55300	0.47100	-11.5
5	0.01075	0.00871	0.47600	0.55600	0.47800	-18.9
6	0.00254	0.00250	0.10100	0.54800	0.45100	-1.5
7	0.03194	0.03380	2.33500	0.55000	0.61000	5.8
8	0.02870	0.02860	2.54000	0.45200	0.51000	-0.3
9	0.03128	0.02970	2.40500	0.52400	0.57200	-5.0
10	0.00269	0.00440	0.48900	0.09800	0.51300	63.3
11	0.00930	0.01106	0.48000	0.48000	2.55500	18.8
12	0.00760	0.00533	0.55500	0.29900	1.64500	-29.8
13	0.01769	0.01885	0.59900	0.99600	0.90700	6.5
14	0.01576	0.01414	0.43800	1.52300	0.13600	-10.2
15	0.01692	0.01590	0.47800	1.48000	0.14400	-6.0

PHL = 0.000036
 AVG PCT ERROR = 14.1

// JOB F 1001 2002 3003 4004 F 2002

FUN

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - LSEST GROUP - CSRD

```
// FOR
*ONE WORD INTEGERS
*LIST ALL
SUBROUTINE FUN(BB)
DIMENSION BB(10)
COMMON KEY,MJM,ND,NF,NFD,NI,NP,PHIZ,SL,B(10),F( 40),G(10),S(10),
1 Y( 40),A(10,10),X(40,16),P(1,10),IPRIN,ILM,MAT,MAR,IPART,
2 FF( 40),KPOIN,NR,NW
DC 1 I=1,ND
DENOM=(1+BB(1)*X(I,1)+BB(2)*X(I,2)+BB(3)*X(I,3))
1 FF(I) = BB(1)*BB(2)*BB(4)*X(I,1)*X(I,2) / DENOM**2
RETURN
END
```

VARIABLE ALLOCATIONS

KEY(IC)=7FFF	MJM(IC)=7FFE	ND(IC)=7FFD	NF(IC)=7FFC
NP(IC)=7FF9	PHIZ(RC)=7FF6	SL(RC)=7FF4	B(RC)=7FF2-7FE0
S(RC)=7F7A-7F68	Y(RC)=7F66-7F18	A(RC)=7F16-7E50	X(RC)=7E4E-7950
ILM(IC)=793A	MAT(IC)=7939	MAR(IC)=7938	IPART(IC)=7937
NR(IC)=78E4	NW(IC)=78E3	DENOM(R)=0000	I(I)=0008

STATEMENT ALLOCATIONS

1 =C058

FEATURES SUPPORTED

ONE WORD INTEGERS

CALLED SUBPROGRAMS

FADD	FMPYX	FLD	FLDX	FSTO	FSTOX	FDVR	FAXI	FLOAT	SUBSC
------	-------	-----	------	------	-------	------	------	-------	-------

INTEGER CONSTANTS

1=C010 2=0011

CORE REQUIREMENTS FOR FUN

COMMON 1822 VARIABLES 16 PROGRAM 116

RELATIVE ENTRY POINT ADDRESS IS 0012 (HEX)

END OF COMPILATION

// DUP

```
*DELETE FUN 2002
CART ID 2002 DB ADDR 2889 DB CNT 0006
```

```
*STCRE WS UA FUN 2002 2002
CART ID 2002 DB ADDR 431F DB CNT 0009
```

// JOB F 1001 2002 3003 4004 F 2002

PART

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - LSEST GROUP - CSRD

```
// FOR
*ONE WORD INTEGERS
*LIST ALL
SUBROUTINE PART
COMMON KEY,MJM,ND,NF,NFD,NI,NP,PHIZ,SL,B(10),F( 40),G(10),S(10),
1 Y( 40),A(10,10),X(40,16),P(1,10),IPRIN,ILM,MAT,MAR,IPART,
2 FF( 40),KPCIN,NR,NW
K=KPOIN
DENOM=(1+ B(1)*X(K,1)+ B(2)*X(K,2)+ B(3)*X(K,3))
P(1,1)= B(2)*B(4)*X(K,1)*X(K,2)*(DENOM-2*B(1)*X(K,1)) / DENOM**3
P(1,2)= B(1)*B(4)*X(K,1)*X(K,2)*(DENOM-2*B(2)*X(K,2)) / DENOM**3
P(1,3)= 2.0*B(1)*B(2)*B(4)*X(K,1)*X(K,2)*X(K,3) /DENOM**3
P(1,4)= B(1)*B(2)*X(K,1)*X(K,2) / DENOM**2
RETURN
END
```

VARIABLE ALLOCATIONS

KEY(IC)=7FFF	MJM(IC)=7FFE	ND(IC)=7FFD	NF(IC)=7FFC
NP(IC)=7FF9	PHIZ(RC)=7FF6	SL(RC)=7FF4	B(RC)=7FF2-7FE0
S(RC)=7F7A-7F68	Y(RC)=7F66-7F18	A(RC)=7F16-7E50	X(RC)=7E4E-7950
ILM(IC)=793A	MAT(IC)=7939	MAR(IC)=7938	IPART(IC)=7937
NR(IC)=78E4	NW(IC)=78E3	DENOM(R)=0000	K(I)=0008

FEATURES SUPPORTED
ONE WORD INTEGERS

CALLED SUBPROGRAMS
 FADD FMPY FMPYX FLD FLDX FSTO FSTOX FSBR FDVR FAXI

REAL CONSTANTS
.200000E 01=0010

INTEGER CONSTANTS
1=C012 2=0013 3=0014

CORE REQUIREMENTS FOR PART
COMMON 1822 VARIABLES 16 PROGRAM 224

RELATIVE ENTRY POINT ADDRESS IS 0015 (HEX)

END OF CCMPILATION

// DUP

```
*DELETE                      PART                      2002
CART ID 2002      DB ADDR 2889      DB CNT 000A
```

```
*STORE                      WS      UA      PART                      2002      2002
CART ID 2002      DB ADDR 4328      DB CNT 0012
```


DEPENDENT

INDEPENDENT

DEPENDENT	INDEPENDENT 1	2	3	4
0.35300E-02	0.48200E 00	0.10000E 00	0.50800E 00	
0.25000E-01	0.24590E 01	0.52700E 00	0.51500E 00	
0.32000E-01	0.24500E 01	0.53000E 00	0.51500E 00	
0.55300E-02	0.47700E 00	0.49400E 00	0.25380E 01	
0.87000E-02	0.51400E 00	0.54000E 00	0.45500E 00	
0.13920E-01	0.47300E 00	0.55200E 00	0.47300E 00	
0.96000E-02	0.47000E 00	0.55800E 00	0.47300E 00	
0.51400E-02	0.10400E 00	0.56200E 00	0.44000E 00	
0.19200E-01	0.45000E 00	0.28400E 01	0.23000E 00	
0.20600E-01	0.40900E 00	0.28100E 01	0.28900E 00	
0.13100E-01	0.48400E 00	0.10750E 01	0.94200E 00	
0.18600E-01	0.35700E 00	0.15900E 01	0.15300E 00	

Mechanism (d) - Non-linear Regression

EXPERIMENTAL DATA

200°C

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.68124E-04 PARAMETERS	SQRT(PHI)/ND= 0.68781E-03 0.41000E 00 0.55000E 00	LAMBDA= 0.10000E-01 0.37000E 00 0.58000E 00	MATRIX
PHI= 0.63375E-04 PARAMETERS	SQRT(PHI)/ND= 0.66340E-03 0.31776E 00 0.46954E 00	LAMBDA= 0.10000E-02 0.34217E 00 0.69656E 00	MATRIX
PHI= 0.61391E-04 PARAMETERS	SQRT(PHI)/ND= 0.65293E-03 0.32173E 00 0.47169E 00	LAMBDA= 0.99999E 00 0.34236E 00 0.70246E 00	MATRIX
PHI= 0.61302E-04 PARAMETERS	SQRT(PHI)/ND= 0.65246E-03 0.32336E 00 0.47182E 00	LAMBDA= 0.99999E 00 0.33664E 00 0.70520E 00	MATRIX
PHI= 0.61297E-04 PARAMETERS	SQRT(PHI)/ND= 0.65243E-03 0.32334E 00 0.47175E 00	LAMBDA= 0.99999E-02 0.33673E 00 0.70525E 00	MATRIX
PHI= 0.61292E-04 PARAMETERS	SQRT(PHI)/ND= 0.65241E-03 0.32332E 00 0.47167E 00	LAMBDA= 0.99999E-02 0.33682E 00 0.70529E 00	MATRIX
PHI= 0.61286E-04 PARAMETERS	SQRT(PHI)/ND= 0.65238E-03 0.32331E 00 0.47160E 00	LAMBDA= 0.99999E-02 0.33690E 00 0.70532E 00	MATRIX
PHI= 0.61281E-04 PARAMETERS	SQRT(PHI)/ND= 0.65235E-03 0.32329E 00 0.47153E 00	LAMBDA= 0.99999E-02 0.33699E 00 0.70536E 00	MATRIX
PHI= 0.61276E-04 PARAMETERS	SQRT(PHI)/ND= 0.65232E-03 0.32328E 00 0.47146E 00	LAMBDA= 0.99999E-02 0.33707E 00 0.70539E 00	MATRIX
PHI= 0.61272E-04 PARAMETERS	SQRT(PHI)/ND= 0.65230E-03 0.32327E 00 0.47139E 00	LAMBDA= 0.99999E-02 0.33716E 00 0.70543E 00	MATRIX
PHI= 0.61267E-04 PARAMETERS	SQRT(PHI)/ND= 0.65228E-03 0.32326E 00 0.47132E 00	LAMBDA= 0.99999E-02 0.33724E 00 0.70545E 00	MATRIX
PHI= 0.61263E-04 PARAMETERS	SQRT(PHI)/ND= 0.65225E-03 0.32325E 00 0.47126E 00	LAMBDA= 0.99999E-02 0.33732E 00 0.70548E 00	MATRIX
PHI= 0.61259E-04 PARAMETERS	SQRT(PHI)/ND= 0.65223E-03 0.32324E 00 0.47119E 00	LAMBDA= 0.99999E-02 0.33740E 00 0.70551E 00	MATRIX
PHI= 0.61255E-04 PARAMETERS	SQRT(PHI)/ND= 0.65221E-03 0.32323E 00 0.47113E 00	LAMBDA= 0.99999E-02 0.33748E 00 0.70553E 00	MATRIX
PHI= 0.61251E-04 PARAMETERS	SQRT(PHI)/ND= 0.65219E-03 0.32322E 00 0.47107E 00	LAMBDA= 0.99999E-02 0.33756E 00 0.70555E 00	MATRIX
PHI= 0.61247E-04 PARAMETERS	SQRT(PHI)/ND= 0.65217E-03 0.32322E 00 0.47101E 00	LAMBDA= 0.99999E-02 0.33763E 00 0.70557E 00	MATRIX
PHI= 0.61243E-04 PARAMETERS	SQRT(PHI)/ND= 0.65215E-03 0.32321E 00 0.47095E 00	LAMBDA= 0.99999E-02 0.33771E 00 0.70558E 00	MATRIX
PHI= 0.61240E-04 PARAMETERS	SQRT(PHI)/ND= 0.65213E-03 0.32321E 00 0.47090E 00	LAMBDA= 0.99999E-02 0.33778E 00 0.70560E 00	MATRIX
PHI= 0.61237E-04 PARAMETERS	SQRT(PHI)/ND= 0.65211E-03 0.32321E 00 0.47084E 00	LAMBDA= 0.99999E-02 0.33786E 00 0.70561E 00	MATRIX
PHI= 0.61233E-04 PARAMETERS	SQRT(PHI)/ND= 0.65209E-03 0.32321E 00 0.47079E 00	LAMBDA= 0.99999E-02 0.33793E 00 0.70562E 00	MATRIX

PHI= 0.61230E-04 PARAMETERS	SQRT(PHI)/ND= 0.65208E-03 0.32321E 00 0.47074E 00	LAMBDA= 0.99999E-02 0.33800E 00 0.70563E 00	MATRIX
PHI= 0.61227E-04 PARAMETERS	SQRT(PHI)/ND= 0.65206E-03 0.32321E 00 0.47069E 00	LAMBDA= 0.99999E-02 0.33807E 00 0.70563E 00	MATRIX
PHI= 0.61224E-04 PARAMETERS	SQRT(PHI)/ND= 0.65205E-03 0.32321E 00 0.47064E 00	LAMBDA= 0.99999E-02 0.33814E 00 0.70564E 00	MATRIX
PHI= 0.61221E-04 PARAMETERS	SQRT(PHI)/ND= 0.65203E-03 0.32321E 00 0.47059E 00	LAMBDA= 0.99999E-02 0.33821E 00 0.70564E 00	MATRIX
PHI= 0.61219E-04 PARAMETERS	SQRT(PHI)/ND= 0.65202E-03 0.32321E 00 0.47055E 00	LAMBDA= 0.99999E-02 0.33828E 00 0.70564E 00	MATRIX
PHI= 0.61216E-04 PARAMETERS	SQRT(PHI)/ND= 0.65200E-03 0.32322E 00 0.47050E 00	LAMBDA= 0.99999E-02 0.33835E 00 0.70564E 00	MATRIX
PHI= 0.61214E-04 PARAMETERS	SQRT(PHI)/ND= 0.65199E-03 0.32322E 00 0.47046E 00	LAMBDA= 0.99999E-02 0.33841E 00 0.70564E 00	MATRIX
PHI= 0.61211E-04 PARAMETERS	SQRT(PHI)/ND= 0.65198E-03 0.32323E 00 0.47042E 00	LAMBDA= 0.99999E-02 0.33848E 00 0.70563E 00	MATRIX
PHI= 0.61209E-04 PARAMETERS	SQRT(PHI)/ND= 0.65197E-03 0.32324E 00 0.47038E 00	LAMBDA= 0.99999E-02 0.33854E 00 0.70563E 00	MATRIX

ALGORITHM TERMINATED

PHI= 0.61209E-04 PARAMETERS	SQRT(PHI)/ND= 0.65197E-03 0.32324E 00 0.47038E 00	LAMBDA= 0.99999E 04 0.33854E 00 0.70563E 00	MATRIX
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DEPENDENT	DIFFERENCE	INDEPENDENT	1	2	3	4
0.27359E-02	0.79404E-03	0.48200E 00	0.10000E 00	0.50800E 00		
0.28284E-01	-0.32849E-02	0.24590E 01	0.52700E 00	0.51500E 00		
0.28380E-01	0.36197E-02	0.24500E 01	0.53000E 00	0.51500E 00		
0.50125E-02	0.51741E-03	0.47700E 00	0.49400E 00	0.25380E 01		
0.12017E-01	-0.33170E-02	0.51400E 00	0.54000E 00	0.45500E 00		
0.11325E-01	0.25940E-02	0.47300E 00	0.55200E 00	0.47300E 00		
0.11349E-01	-0.17497E-02	0.47000E 00	0.55800E 00	0.47300E 00		
0.29952E-02	0.21447E-02	0.10400E 00	0.56200E 00	0.44000E 00		
0.20935E-01	-0.17351E-02	0.45000E 00	0.28400E 01	0.23000E 00		
0.18935E-01	0.16641E-02	0.40900E 00	0.28100E 01	0.28900E 00		
0.14224E-01	-0.11242E-02	0.48400E 00	0.10750E 01	0.94200E 00		
0.16604E-01	0.19950E-02	0.35700E 00	0.15900E 01	0.15300E 00		

CORRELATION MATRIX

1.000			
0.534	1.000		
0.737	0.869	1.000	
0.895	0.826	0.863	1.000

29 STEPS

DEPENDENT

INDEPENDENT
1

2

3

0.35300E-02
0.25000E-01
0.32000E-01
0.55300E-02
0.87000E-02
0.13920E-01
0.96000E-02
0.51400E-02
0.19200E-01
0.20600E-01
0.13100E-01
0.18600E-01

.1749
.01456ms

0.48200E 00
0.24590E 01
0.24500E 01
0.47700E 00
0.51400E 00
0.47300E 00
0.47000E 00
0.10400E 00
0.45000E 00
0.40900E 00
0.48400E 00
0.35700E 00

0.10000E 00
0.52700E 00
0.53000E 00
0.49400E 00
0.54000E 00
0.55200E 00
0.55800E 00
0.56200E 00
0.28400E 01
0.28100E 01
0.10750E 01
0.15900E 01

0.50800E 00
0.51500E 00
0.51500E 00
0.25380E 01
0.45500E 00
0.47300E 00
0.47300E 00
0.44000E 00
0.23000E 00
0.28900E 00
0.94200E 00
0.15300E 00

MATRIX 1 IS A + SL*D
MATRIX 2 IS A + SL*I
MATRIX 3 IS A + SL*D-1

Mechanism (d)
Experimental Data, Non-Linear Regression
Initial Constants from Linear Regression
200°F

PHI= 0.64066E-04 PARAMETERS	SQRT(PHI)/ND= 0.66701E-03 0.40000E 00	0.58000E 00	LAMBDA= 0.10000E-01 0.50000E 00	0.61000E 00	MATR
PHI= 0.63376E-04 PARAMETERS	SQRT(PHI)/ND= 0.66341E-03 0.38767E 00	0.56694E 00	LAMBDA= 0.10000E 00 0.48186E 00	0.62306E 00	MATR
PHI= 0.62974E-04 PARAMETERS	SQRT(PHI)/ND= 0.66130E-03 0.37828E 00	0.55394E 00	LAMBDA= 0.99999E-01 0.46330E 00	0.63475E 00	MATR
PHI= 0.61717E-04 PARAMETERS	SQRT(PHI)/ND= 0.65467E-03 0.34372E 00	0.50589E 00	LAMBDA= 0.99999E-02 0.47323E 00	0.68300E 00	MATR
PHI= 0.61256E-04 PARAMETERS	SQRT(PHI)/ND= 0.65221E-03 0.34328E 00	0.50654E 00	LAMBDA= 0.99999E-01 0.48744E 00	0.69064E 00	MATR
PHI= 0.61101E-04 PARAMETERS	SQRT(PHI)/ND= 0.65139E-03 0.34400E 00	0.50864E 00	LAMBDA= 0.99999E 00 0.49576E 00	0.69266E 00	MATR
PHI= 0.61081E-04 PARAMETERS	SQRT(PHI)/ND= 0.65128E-03 0.34438E 00	0.51029E 00	LAMBDA= 0.99999E 00 0.50352E 00	0.69411E 00	MATR
PHI= 0.61058E-04 PARAMETERS	SQRT(PHI)/ND= 0.65116E-03 0.34460E 00	0.51081E 00	LAMBDA= 0.99999E 01 0.50534E 00	0.69453E 00	MATR
PHI= 0.61041E-04 PARAMETERS	SQRT(PHI)/ND= 0.65107E-03 0.34478E 00	0.51128E 00	LAMBDA= 0.99999E 01 0.50707E 00	0.69491E 00	MATR
PHI= 0.61031E-04 PARAMETERS	SQRT(PHI)/ND= 0.65102E-03 0.34494E 00	0.51173E 00	LAMBDA= 0.99999E 01 0.50872E 00	0.69526E 00	MATR
PHI= 0.61025E-04 PARAMETERS	SQRT(PHI)/ND= 0.65098E-03 0.34509E 00	0.51214E 00	LAMBDA= 0.99999E 01 0.51031E 00	0.69557E 00	MATR
PHI= 0.61022E-04 PARAMETERS	SQRT(PHI)/ND= 0.65097E-03 0.34521E 00	0.51254E 00	LAMBDA= 0.99999E 01 0.51183E 00	0.69586E 00	MATR
PHI= 0.61019E-04 PARAMETERS	SQRT(PHI)/ND= 0.65095E-03 0.34523E 00	0.51256E 00	LAMBDA= 0.99999E 00 0.51184E 00	0.69589E 00	MATR
PHI= 0.60997E-04 PARAMETERS	SQRT(PHI)/ND= 0.65084E-03 0.34540E 00	0.51276E 00	LAMBDA= 0.99999E-01 0.51195E 00	0.69610E 00	MATR
PHI= 0.60946E-04 PARAMETERS	SQRT(PHI)/ND= 0.65056E-03 0.34561E 00	0.51374E 00	LAMBDA= 0.99999E-02 0.51262E 00	0.69694E 00	MATR
PHI= 0.60933E-04 PARAMETERS	SQRT(PHI)/ND= 0.65050E-03 0.34550E 00	0.51438E 00	LAMBDA= 0.99999E-02 0.51319E 00	0.69741E 00	MATR
PHI= 0.60930E-04 PARAMETERS	SQRT(PHI)/ND= 0.65048E-03 0.34532E 00	0.51484E 00	LAMBDA= 0.99999E-02 0.51370E 00	0.69772E 00	MATR
PHI= 0.60929E-04 PARAMETERS	SQRT(PHI)/ND= 0.65047E-03 0.34513E 00	0.51518E 00	LAMBDA= 0.99999E-02 0.51418E 00	0.69796E 00	MATR
PHI= 0.60929E-04 PARAMETERS	SQRT(PHI)/ND= 0.65047E-03 0.34513E 00	0.51520E 00	LAMBDA= 0.99999E-03 0.51419E 00	0.69799E 00	MATR
PHI= 0.60926E-04 PARAMETERS	SQRT(PHI)/ND= 0.65046E-03 0.34502E 00	0.51536E 00	LAMBDA= 0.99999E-04 0.51422E 00	0.69818E 00	MATR

PHI= 0.60923E-04 PARAMETERS	SQRT(PHI)/ND= 0.65044E-03 0.34429E 00 0.51568E 00	LAMBDA= 0.99999E-05 0.51450E 00 0.69901E 00	MATRI
PHI= 0.60923E-04 PARAMETERS	SQRT(PHI)/ND= 0.65044E-03 0.34426E 00 0.51573E 00	LAMBDA= 0.99999E-04 0.51453E 00 0.69911E 00	MATRI
PHI= 0.60923E-04 PARAMETERS	SQRT(PHI)/ND= 0.65044E-03 0.34421E 00 0.51576E 00	LAMBDA= 0.99999E-04 0.51456E 00 0.69920E 00	MATRI
PHI= 0.60922E-04 PARAMETERS	SQRT(PHI)/ND= 0.65044E-03 0.34421E 00 0.51576E 00	LAMBDA= 0.99999E-01 0.51456E 00 0.69920E 00	MATRI

ALGORITHM TERMINATED

PHI= 0.60922E-04 PARAMETERS	SQRT(PHI)/ND= 0.65044E-03 0.34421E 00 0.51576E 00	LAMBDA= 0.10000E 04 0.51456E 00 0.69920E 00	MATRI
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SINGULAR MATRIX

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3
		1		
0.27356E-02	0.79432E-03	0.48200E 00	0.10000E 00	0.50800E 00
0.28321E-01	-0.33218E-02	0.24590E 01	0.52700E 00	0.51500E 00
0.28415E-01	0.35842E-02	0.24500E 01	0.53000E 00	0.51500E 00
0.39393E-02	0.15906E-02	0.47700E 00	0.49400E 00	0.25380E 01
0.12069E-01	-0.33696E-02	0.51400E 00	0.54000E 00	0.45500E 00
0.11335E-01	0.25842E-02	0.47300E 00	0.55200E 00	0.47300E 00
0.11358E-01	-0.17585E-02	0.47000E 00	0.55800E 00	0.47300E 00
0.30118E-02	0.21281E-02	0.10400E 00	0.56200E 00	0.44000E 00
0.21161E-01	-0.19616E-02	0.45000E 00	0.28400E 01	0.23000E 00
0.19019E-01	0.15803E-02	0.40900E 00	0.28100E 01	0.28900E 00
0.13274E-01	-0.17466E-03	0.48400E 00	0.10750E 01	0.94200E 00
0.17239E-01	0.13602E-02	0.35700E 00	0.15900E 01	0.15300E 00

CORRELATION MATRIX

1.000			
0.514	1.000		
0.748	0.890	1.000	
0.897	0.809	0.888	1.000

24 STEPS

DEPENDENT	INDEPENDENT		
	1	2	3
0.35300E-02	0.48200E 00	0.10000E 00	0.50800E 00
0.25000E-01	0.24590E 01	0.52700E 00	0.51500E 00
0.32000E-01	0.24500E 01	0.53000E 00	0.51500E 00
0.55300E-02	0.47700E 00	0.49400E 00	0.25380E 01
0.87000E-02	0.51400E 00	0.54000E 00	0.45500E 00
0.13920E-01	0.47300E 00	0.55200E 00	0.47300E 00
0.96000E-02	0.47000E 00	0.55800E 00	0.47300E 00
0.51400E-02	0.10400E 00	0.56200E 00	0.44000E 00
0.19200E-01	0.45000E 00	0.28400E 01	0.23000E 00
0.20600E-01	0.40900E 00	0.28100E 01	0.28900E 00
0.13100E-01	0.48400E 00	0.10750E 01	0.94200E 00
0.18600E-01	0.35700E 00	0.15900E 01	0.15300E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.61134E-03 PARAMETERS	SQRT(PHI)/ND= 0.20604E-02 0.48000E 00	0.70000E 00	LAMBDA= 0.10000E-01 0.60000E 00	0.73000E 00	MATRI
PHI= 0.71459E-04 PARAMETERS	SQRT(PHI)/ND= 0.70444E-03 0.37253E 00	0.55059E 00	LAMBDA= 0.99999E-02 0.67862E 00	0.65477E 00	MATRI
PHI= 0.68974E-04 PARAMETERS	SQRT(PHI)/ND= 0.69209E-03 0.37594E 00	0.56174E 00	LAMBDA= 0.99999E 00 0.71803E 00	0.66169E 00	MATRI
PHI= 0.68333E-04 PARAMETERS	SQRT(PHI)/ND= 0.68886E-03 0.37802E 00	0.57091E 00	LAMBDA= 0.99999E 00 0.75398E 00	0.66655E 00	MATRI
PHI= 0.67899E-04 PARAMETERS	SQRT(PHI)/ND= 0.68667E-03 0.37900E 00	0.57343E 00	LAMBDA= 0.99999E 01 0.76243E 00	0.66811E 00	MATRI
PHI= 0.67578E-04 PARAMETERS	SQRT(PHI)/ND= 0.68505E-03 0.37986E 00	0.57579E 00	LAMBDA= 0.99999E 01 0.77039E 00	0.66952E 00	MATRI
PHI= 0.67345E-04 PARAMETERS	SQRT(PHI)/ND= 0.68386E-03 0.38062E 00	0.57801E 00	LAMBDA= 0.99999E 01 0.77793E 00	0.67079E 00	MATR
PHI= 0.67178E-04 PARAMETERS	SQRT(PHI)/ND= 0.68302E-03 0.38129E 00	0.58009E 00	LAMBDA= 0.99999E 01 0.78510E 00	0.67195E 00	MATR
PHI= 0.67065E-04 PARAMETERS	SQRT(PHI)/ND= 0.68244E-03 0.38188E 00	0.58206E 00	LAMBDA= 0.99999E 01 0.79195E 00	0.67300E 00	MATR
PHI= 0.66993E-04 PARAMETERS	SQRT(PHI)/ND= 0.68207E-03 0.38241E 00	0.58393E 00	LAMBDA= 0.99999E 01 0.79853E 00	0.67396E 00	MATR
PHI= 0.66954E-04 PARAMETERS	SQRT(PHI)/ND= 0.68187E-03 0.38289E 00	0.58571E 00	LAMBDA= 0.99999E 01 0.80486E 00	0.67485E 00	MATR
PHI= 0.66940E-04 PARAMETERS	SQRT(PHI)/ND= 0.68180E-03 0.38332E 00	0.58741E 00	LAMBDA= 0.99999E 01 0.81098E 00	0.67567E 00	MATR
PHI= 0.66914E-04 PARAMETERS	SQRT(PHI)/ND= 0.68167E-03 0.38338E 00	0.58748E 00	LAMBDA= 0.99999E 00 0.81102E 00	0.67574E 00	MATR
PHI= 0.66707E-04 PARAMETERS	SQRT(PHI)/ND= 0.68062E-03 0.38384E 00	0.58811E 00	LAMBDA= 0.99999E-01 0.81132E 00	0.67639E 00	MATR
PHI= 0.66121E-04 PARAMETERS	SQRT(PHI)/ND= 0.67762E-03 0.38468E 00	0.59185E 00	LAMBDA= 0.99999E-02 0.81333E 00	0.67890E 00	MATR
PHI= 0.65938E-04 PARAMETERS	SQRT(PHI)/ND= 0.67668E-03 0.38447E 00	0.59455E 00	LAMBDA= 0.99999E-02 0.81501E 00	0.68008E 00	MATR
PHI= 0.65858E-04 PARAMETERS	SQRT(PHI)/ND= 0.67627E-03 0.38400E 00	0.59666E 00	LAMBDA= 0.99999E-02 0.81651E 00	0.68069E 00	MATR
PHI= 0.65820E-04 PARAMETERS	SQRT(PHI)/ND= 0.67608E-03 0.38352E 00	0.59838E 00	LAMBDA= 0.99999E-02 0.81791E 00	0.68103E 00	MATR
PHI= 0.65803E-04 PARAMETERS	SQRT(PHI)/ND= 0.67599E-03 0.38313E 00	0.59982E 00	LAMBDA= 0.99999E-02 0.81926E 00	0.68122E 00	MATR
PHI= 0.65800E-04 PARAMETERS	SQRT(PHI)/ND= 0.67597E-03 0.38284E 00	0.60104E 00	LAMBDA= 0.99999E-02 0.82055E 00	0.68133E 00	MATR

PHI= 0.65799E-04 PARAMETERS	SQRT(PHI)/ND= 0.67597E-03 0.38284E 00 0.60119E 00	LAMBDA= 0.99999E-01 0.82069E 00 0.68137E 00	MATRI
PHI= 0.65799E-04 PARAMETERS	SQRT(PHI)/ND= 0.67597E-03 0.38284E 00 0.60132E 00	LAMBDA= 0.99999E-01 0.82083E 00 0.68141E 00	MATRI
PHI= 0.65798E-04 PARAMETERS	SQRT(PHI)/ND= 0.67597E-03 0.38283E 00 0.60146E 00	LAMBDA= 0.99999E-01 0.82096E 00 0.68144E 00	MATRI
PHI= 0.65798E-04 PARAMETERS	SQRT(PHI)/ND= 0.67597E-03 0.38282E 00 0.60159E 00	LAMBDA= 0.99999E-01 0.82110E 00 0.68147E 00	MATRI
PHI= 0.65798E-04 PARAMETERS	SQRT(PHI)/ND= 0.67596E-03 0.38282E 00 0.60160E 00	LAMBDA= 0.99999E-02 0.82110E 00 0.68147E 00	MATRI
PHI= 0.65798E-04 PARAMETERS	SQRT(PHI)/ND= 0.67596E-03 0.38282E 00 0.60160E 00	LAMBDA= 0.99999E-02 0.82110E 00 0.68148E 00	MATRI

ALGORITHM CONVERGED

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3
		1		
0.27394E-02	0.79059E-03	0.48200E 00	0.10000E 00	0.50800E 00
0.28291E-01	-0.32912E-02	0.24590E 01	0.52700E 00	0.51500E 00
0.28382E-01	0.36171E-02	0.24500E 01	0.53000E 00	0.51500E 00
0.29120E-02	0.26179E-02	0.47700E 00	0.49400E 00	0.25380E 01
0.12128E-01	-0.34282E-02	0.51400E 00	0.54000E 00	0.45500E 00
0.11333E-01	0.25866E-02	0.47300E 00	0.55200E 00	0.47300E 00
0.11354E-01	-0.17544E-02	0.47000E 00	0.55800E 00	0.47300E 00
0.30327E-02	0.21072E-02	0.10400E 00	0.56200E 00	0.47000E 00
0.21286E-01	-0.20869E-02	0.45000E 00	0.28400E 01	0.23000E 00
0.18961E-01	0.16389E-02	0.40900E 00	0.28100E 01	0.28900E 00
0.12029E-01	0.10706E-02	0.48400E 00	0.10750E 01	0.94200E 00
0.18095E-01	0.50412E-03	0.35700E 00	0.15900E 01	0.15300E 00

CORRELATION MATRIX

1.000			
0.478	1.000		
0.754	0.899	1.000	
0.901	0.780	0.906	1.000

25 STEPS

DEPENDENT

INDEPENDENT

0.35300E-02
 0.25000E-01
 0.32000E-01
 0.55300E-02
 0.87000E-02
 0.13920E-01
 0.96000E-02
 0.51400E-02
 0.19200E-01
 0.20600E-01
 0.13100E-01
 0.18600E-01

0.48200E 00
 0.24590E 01
 0.24500E 01
 0.47700E 00
 0.51400E 00
 0.47300E 00
 0.47000E 00
 0.10400E 00
 0.45000E 00
 0.40900E 00
 0.48400E 00
 0.35700E 00

2

3

0.10000E 00
 0.52700E 00
 0.53000E 00
 0.49400E 00
 0.54000E 00
 0.55200E 00
 0.55800E 00
 0.56200E 00
 0.28400E 01
 0.28100E 01
 0.10750E 01
 0.15900E 01

0.50800E 00
 0.51500E 00
 0.51500E 00
 0.25380E 01
 0.45500E 00
 0.47300E 00
 0.47300E 00
 0.44000E 00
 0.23000E 00
 0.28900E 00
 0.94200E 00
 0.15300E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.80504E-04 PARAMETERS	SQRT(PHI)/ND= 0.74770E-03 0.38000E 00	0.68000E 00	LAMBDA= 0.10000E-01 0.82000E 00	0.68000E 00	MATRIX
PHI= 0.72323E-04 PARAMETERS	SQRT(PHI)/ND= 0.70869E-03 0.38233E 00	0.61002E 00	LAMBDA= 0.10000E 00 0.87928E 00	0.66402E 00	MATRIX
PHI= 0.72144E-04 PARAMETERS	SQRT(PHI)/ND= 0.70781E-03 0.38678E 00	0.61659E 00	LAMBDA= 0.10000E 01 0.92205E 00	0.66898E 00	MATRIX
PHI= 0.71679E-04 PARAMETERS	SQRT(PHI)/ND= 0.70553E-03 0.38809E 00	0.61922E 00	LAMBDA= 0.10000E 02 0.93213E 00	0.67069E 00	MATRIX
PHI= 0.71346E-04 PARAMETERS	SQRT(PHI)/ND= 0.70388E-03 0.38926E 00	0.62168E 00	LAMBDA= 0.99999E 01 0.94165E 00	0.67223E 00	MATRIX
PHI= 0.71114E-04 PARAMETERS	SQRT(PHI)/ND= 0.70274E-03 0.39032E 00	0.62399E 00	LAMBDA= 0.99999E 01 0.95068E 00	0.67363E 00	MATRIX
PHI= 0.70960E-04 PARAMETERS	SQRT(PHI)/ND= 0.70198E-03 0.39126E 00	0.62616E 00	LAMBDA= 0.99999E 01 0.95928E 00	0.67489E 00	MATRIX
PHI= 0.70868E-04 PARAMETERS	SQRT(PHI)/ND= 0.70152E-03 0.39212E 00	0.62822E 00	LAMBDA= 0.99999E 01 0.96753E 00	0.67604E 00	MATRIX
PHI= 0.70823E-04 PARAMETERS	SQRT(PHI)/ND= 0.70130E-03 0.39289E 00	0.63018E 00	LAMBDA= 0.99999E 01 0.97545E 00	0.67710E 00	MATRIX
PHI= 0.70816E-04 PARAMETERS	SQRT(PHI)/ND= 0.70126E-03 0.39360E 00	0.63205E 00	LAMBDA= 0.99999E 01 0.98309E 00	0.67807E 00	MATRIX
PHI= 0.70811E-04 PARAMETERS	SQRT(PHI)/ND= 0.70124E-03 0.39369E 00	0.63228E 00	LAMBDA= 0.99999E 02 0.98399E 00	0.67819E 00	MATRIX
PHI= 0.70806E-04 PARAMETERS	SQRT(PHI)/ND= 0.70122E-03 0.39378E 00	0.63251E 00	LAMBDA= 0.99999E 02 0.98488E 00	0.67831E 00	MATRIX
PHI= 0.70803E-04 PARAMETERS	SQRT(PHI)/ND= 0.70120E-03 0.39387E 00	0.63274E 00	LAMBDA= 0.99999E 02 0.98576E 00	0.67844E 00	MATRIX
PHI= 0.70799E-04 PARAMETERS	SQRT(PHI)/ND= 0.70118E-03 0.39395E 00	0.63297E 00	LAMBDA= 0.99999E 02 0.98664E 00	0.67856E 00	MATRIX
PHI= 0.70796E-04 PARAMETERS	SQRT(PHI)/ND= 0.70117E-03 0.39404E 00	0.63319E 00	LAMBDA= 0.99999E 02 0.98752E 00	0.67867E 00	MATRIX
PHI= 0.70794E-04 PARAMETERS	SQRT(PHI)/ND= 0.70116E-03 0.39413E 00	0.63342E 00	LAMBDA= 0.99999E 02 0.98839E 00	0.67879E 00	MATRIX
PHI= 0.70792E-04 PARAMETERS	SQRT(PHI)/ND= 0.70115E-03 0.39421E 00	0.63364E 00	LAMBDA= 0.99999E 02 0.98925E 00	0.67891E 00	MATRIX
PHI= 0.70791E-04 PARAMETERS	SQRT(PHI)/ND= 0.70114E-03 0.39429E 00	0.63386E 00	LAMBDA= 0.99999E 02 0.99012E 00	0.67902E 00	MATRIX
PHI= 0.70790E-04 PARAMETERS	SQRT(PHI)/ND= 0.70114E-03 0.39438E 00	0.63408E 00	LAMBDA= 0.99999E 02 0.99097E 00	0.67914E 00	MATRIX
PHI= 0.70789E-04 PARAMETERS	SQRT(PHI)/ND= 0.70113E-03 0.39446E 00	0.63430E 00	LAMBDA= 0.99999E 02 0.99183E 00	0.67925E 00	MATRIX

PHI= 0.70789E-04 PARAMETERS	SQRT(PHI)/ND= 0.70113E-03 0.39454E 00	0.63452E 00	LAMBDA= 0.99999E 02 0.99268E 00	0.67936E 00	MATRI
PHI= 0.70789E-04 PARAMETERS	SQRT(PHI)/ND= 0.70113E-03 0.39455E 00	0.63454E 00	LAMBDA= 0.99999E 03 0.99276E 00	0.67937E 00	MATRI
PHI= 0.70789E-04 PARAMETERS	SQRT(PHI)/ND= 0.70113E-03 0.39456E 00	0.63456E 00	LAMBDA= 0.99999E 03 0.99285E 00	0.67939E 00	MATRI
PHI= 0.70789E-04 PARAMETERS	SQRT(PHI)/ND= 0.70113E-03 0.39456E 00	0.63458E 00	LAMBDA= 0.99999E 03 0.99294E 00	0.67940E 00	MATRI
PHI= 0.70789E-04 PARAMETERS	SQRT(PHI)/ND= 0.70113E-03 0.39457E 00	0.63460E 00	LAMBDA= 0.99999E 03 0.99302E 00	0.67941E 00	MATRI

ALGORITHM TERMINATED

PHI= 0.70789E-04 PARAMETERS	SQRT(PHI)/ND= 0.70113E-03 0.39457E 00	0.63460E 00	LAMBDA= 0.10000E 04 0.99302E 00	0.67941E 00	MATRI
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SINGULAR MATRIX

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3
		1		
0.26529E-02	0.87704E-03	0.48200E 00	0.10000E 00	0.50800E 00
0.27799E-01	-0.27997E-02	0.24590E 01	0.52700E 00	0.51500E 00
0.27888E-01	0.41116E-02	0.24500E 01	0.53000E 00	0.51500E 00
0.24781E-02	0.30518E-02	0.47700E 00	0.49400E 00	0.25380E 01
0.11836E-01	-0.31366E-02	0.51400E 00	0.54000E 00	0.45500E 00
0.11031E-01	0.28885E-02	0.47300E 00	0.55200E 00	0.47300E 00
0.11051E-01	-0.14517E-02	0.47000E 00	0.55800E 00	0.47300E 00
0.29542E-02	0.21857E-02	0.10400E 00	0.56200E 00	0.44000E 00
0.21123E-01	-0.19235E-02	0.45000E 00	0.28400E 01	0.23000E 00
0.18722E-01	0.18776E-02	0.40900E 00	0.28100E 01	0.28900E 00
0.11221E-01	0.18787E-02	0.48400E 00	0.10750E 01	0.94200E 00
0.18226E-01	0.37394E-03	0.35700E 00	0.15900E 01	0.15300E 00

CORRELATION MATRIX

1.000			
0.473	1.000		
0.759	0.902	1.000	
0.906	0.769	0.911	1.000

25 STEPS

DEPENDENT

INDEPENDENT

2

3

4

0.35300E-02	0.48200E 00	0.10000E 00	0.50800E 00
0.25000E-01	0.24590E 01	0.52700E 00	0.51500E 00
0.32000E-01	0.24500E 01	0.53000E 00	0.51500E 00
0.55300E-02	0.47700E 00	0.49400E 00	0.25380E 01
0.87000E-02	0.51400E 00	0.54000E 00	0.45500E 00
0.13920E-01	0.47300E 00	0.55200E 00	0.47300E 00
0.96000E-02	0.47000E 00	0.55800E 00	0.47300E 00
0.51400E-02	0.10400E 00	0.56200E 00	0.44000E 00
0.19200E-01	0.45000E 00	0.28400E 01	0.23000E 00
0.20600E-01	0.40900E 00	0.28100E 01	0.28900E 00
0.13100E-01	0.48400E 00	0.10750E 01	0.94200E 00
0.18600E-01	0.35700E 00	0.15900E 01	0.15300E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.43619E-03 PARAMETERS	SQRT(PHI)/ND= 0.17404E-02 0.32000E 00	0.46000E 00	LAMBDA= 0.10000E-01 0.40000E 00	0.49000E 00	MATRIX
PHI= 0.64895E-04 PARAMETERS	SQRT(PHI)/ND= 0.67131E-03 0.32880E 00	0.49037E 00	LAMBDA= 0.10000E-02 0.37376E 00	0.71858E 00	MATRIX
PHI= 0.62699E-04 PARAMETERS	SQRT(PHI)/ND= 0.65985E-03 0.31929E 00	0.47025E 00	LAMBDA= 0.10000E-03 0.34726E 00	0.73018E 00	MATRIX
PHI= 0.62200E-04 PARAMETERS	SQRT(PHI)/ND= 0.65722E-03 0.31763E 00	0.46617E 00	LAMBDA= 0.99999E 00 0.33282E 00	0.72718E 00	MATRIX
PHI= 0.62058E-04 PARAMETERS	SQRT(PHI)/ND= 0.65647E-03 0.31713E 00	0.46512E 00	LAMBDA= 0.99999E 01 0.32947E 00	0.72630E 00	MATRIX
PHI= 0.61961E-04 PARAMETERS	SQRT(PHI)/ND= 0.65596E-03 0.31670E 00	0.46417E 00	LAMBDA= 0.99999E 01 0.32630E 00	0.72552E 00	MATRIX
PHI= 0.61898E-04 PARAMETERS	SQRT(PHI)/ND= 0.65563E-03 0.31631E 00	0.46328E 00	LAMBDA= 0.99999E 01 0.32329E 00	0.72483E 00	MATRIX
PHI= 0.61862E-04 PARAMETERS	SQRT(PHI)/ND= 0.65543E-03 0.31597E 00	0.46245E 00	LAMBDA= 0.99999E 01 0.32040E 00	0.72420E 00	MATRIX
PHI= 0.61846E-04 PARAMETERS	SQRT(PHI)/ND= 0.65535E-03 0.31566E 00	0.46167E 00	LAMBDA= 0.99999E 01 0.31762E 00	0.72364E 00	MATRIX
PHI= 0.61843E-04 PARAMETERS	SQRT(PHI)/ND= 0.65533E-03 0.31562E 00	0.46158E 00	LAMBDA= 0.99999E 02 0.31730E 00	0.72357E 00	MATRIX
PHI= 0.61841E-04 PARAMETERS	SQRT(PHI)/ND= 0.65532E-03 0.31558E 00	0.46149E 00	LAMBDA= 0.99999E 02 0.31697E 00	0.72350E 00	MATRIX
PHI= 0.61839E-04 PARAMETERS	SQRT(PHI)/ND= 0.65531E-03 0.31554E 00	0.46140E 00	LAMBDA= 0.99999E 02 0.31665E 00	0.72343E 00	MATRIX
PHI= 0.61837E-04 PARAMETERS	SQRT(PHI)/ND= 0.65530E-03 0.31551E 00	0.46130E 00	LAMBDA= 0.99999E 02 0.31633E 00	0.72337E 00	MATRIX
PHI= 0.61835E-04 PARAMETERS	SQRT(PHI)/ND= 0.65529E-03 0.31547E 00	0.46121E 00	LAMBDA= 0.99999E 02 0.31601E 00	0.72330E 00	MATRIX
PHI= 0.61834E-04 PARAMETERS	SQRT(PHI)/ND= 0.65529E-03 0.31543E 00	0.46112E 00	LAMBDA= 0.99999E 02 0.31570E 00	0.72323E 00	MATRIX
PHI= 0.61833E-04 PARAMETERS	SQRT(PHI)/ND= 0.65528E-03 0.31540E 00	0.46104E 00	LAMBDA= 0.99999E 02 0.31538E 00	0.72317E 00	MATRIX
PHI= 0.61832E-04 PARAMETERS	SQRT(PHI)/ND= 0.65528E-03 0.31536E 00	0.46095E 00	LAMBDA= 0.99999E 02 0.31507E 00	0.72310E 00	MATRIX
PHI= 0.61832E-04 PARAMETERS	SQRT(PHI)/ND= 0.65527E-03 0.31532E 00	0.46086E 00	LAMBDA= 0.99999E 02 0.31475E 00	0.72304E 00	MATRIX
PHI= 0.61831E-04 PARAMETERS	SQRT(PHI)/ND= 0.65527E-03 0.31529E 00	0.46077E 00	LAMBDA= 0.99999E 02 0.31444E 00	0.72297E 00	MATRIX
PHI= 0.61831E-04 PARAMETERS	SQRT(PHI)/ND= 0.65527E-03 0.31525E 00	0.46069E 00	LAMBDA= 0.99999E 02 0.31413E 00	0.72291E 00	MATRIX

PHI= 0.61831E-04 SQRT(PHI)/ND= 0.65527E-03 LAMBDA= 0.99999E 02 MATRIX
PARAMETERS 0.31522E 00 0.46060E 00 0.31382E 00 0.72285E 00

PHI= 0.61831E-04 SQRT(PHI)/ND= 0.65527E-03 LAMBDA= 0.99999E 03 MATRIX
PARAMETERS 0.31522E 00 0.46059E 00 0.31379E 00 0.72284E 00

ALGORITHM TERMINATED

PHI= 0.61831E-04 SQRT(PHI)/ND= 0.65527E-03 LAMBDA= 0.10000E 04 MATRIX
PARAMETERS 0.31522E 00 0.46059E 00 0.31379E 00 0.72284E 00

SINGULAR MATRIX

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3	4
		1			
0.27454E-02	0.78456E-03	0.48200E 00	0.10000E 00	0.50800E 00	
0.28631E-01	-0.36319E-02	0.24590E 01	0.52700E 00	0.51500E 00	
0.28727E-01	0.32720E-02	0.24500E 01	0.53000E 00	0.51500E 00	
0.52310E-02	0.29899E-03	0.47700E 00	0.49400E 00	0.25380E 01	
0.12069E-01	-0.33699E-02	0.51400E 00	0.54000E 00	0.45500E 00	
0.11379E-01	0.25404E-02	0.47300E 00	0.55200E 00	0.47300E 00	
0.11403E-01	-0.18035E-02	0.47000E 00	0.55800E 00	0.47300E 00	
0.30009E-02	0.21390E-02	0.10400E 00	0.56200E 00	0.44000E 00	
0.21085E-01	-0.18855E-02	0.45000E 00	0.28400E 01	0.23000E 00	
0.19086E-01	0.15137E-02	0.40900E 00	0.28100E 01	0.28900E 00	
0.14459E-01	-0.13595E-02	0.48400E 00	0.10750E 01	0.94200E 00	
0.16626E-01	0.19736E-02	0.35700E 00	0.15900E 01	0.15300E 00	

CORRELATION MATRIX

1.000			
0.544	1.000		
0.737	0.867	1.000	
0.897	0.830	0.859	1.000

22 STEPS

DEPENDENT	INDEPENDENT	1	2	3
0.35300E-02	0.48200E 00	0.10000E 00	0.50800E 00	0.50800E 00
0.25000E-01	0.24590E 01	0.52700E 00	0.51500E 00	0.51500E 00
0.32000E-01	0.24500E 01	0.53000E 00	0.51500E 00	0.51500E 00
0.55300E-02	0.47700E 00	0.49400E 00	0.25380E 01	0.25380E 01
0.87000E-02	0.51400E 00	0.54000E 00	0.45500E 00	0.45500E 00
0.13920E-01	0.47300E 00	0.55200E 00	0.47300E 00	0.47300E 00
0.96000E-02	0.47000E 00	0.55800E 00	0.47300E 00	0.47300E 00
0.51400E-02	0.10400E 00	0.56200E 00	0.44000E 00	0.44000E 00
0.19200E-01	0.45000E 00	0.28400E 01	0.23000E 00	0.23000E 00
0.20600E-01	0.40900E 00	0.28100E 01	0.28900E 00	0.28900E 00
0.13100E-01	0.48400E 00	0.10750E 01	0.94200E 00	0.94200E 00
0.18600E-01	0.35700E 00	0.15900E 01	0.15300E 00	0.15300E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.61826E-04 Sqrt(PHI)/ND= 0.65524E-03 LAMBDA= 0.10000E-01 MATRIX
 PARAMETERS 0.31000E 00 0.46000E 00 0.31000E 00 0.72000E 00 00

PHI= 0.61816E-04 Sqrt(PHI)/ND= 0.65519E-03 LAMBDA= 0.10000E 02 MATRIX
 PARAMETERS 0.31027E 00 0.45976E 00 0.30883E 00 0.72026E 00 00

ALGORITHM TERMINATED

PHI= 0.61816E-04 Sqrt(PHI)/ND= 0.65519E-03 LAMBDA= 0.10000E 04 MATRIX
 PARAMETERS 0.31027E 00 0.45976E 00 0.30883E 00 0.72026E 00 00

SINGULAR MATRIX

DEPENDENT	DIFFERENCE	INDEPENDENT	1	2	3
0.27077E-02	0.82229E-03	0.48200E 00	0.10000E 00	0.50800E 00	0.50800E 00
0.28425E-01	-0.34252E-02	0.24590E 01	0.52700E 00	0.51500E 00	0.51500E 00
0.28519E-01	0.34803E-02	0.24500E 01	0.53000E 00	0.51500E 00	0.51500E 00
0.51944E-02	0.33555E-03	0.47700E 00	0.49400E 00	0.25380E 01	0.25380E 01
0.11896E-01	-0.31969E-02	0.51400E 00	0.54000E 00	0.45500E 00	0.45500E 00
0.11215E-01	0.27049E-02	0.47300E 00	0.55200E 00	0.47300E 00	0.47300E 00
0.11238E-01	-0.16385E-02	0.47000E 00	0.55800E 00	0.47300E 00	0.47300E 00
0.29510E-02	0.21889E-02	0.10400E 00	0.56200E 00	0.44000E 00	0.44000E 00
0.20737E-01	-0.15372E-02	0.45000E 00	0.28400E 01	0.23000E 00	0.23000E 00
0.18772E-01	0.18276E-02	0.40900E 00	0.28100E 01	0.28900E 00	0.28900E 00
0.14272E-01	-0.11729E-02	0.48400E 00	0.10750E 01	0.94200E 00	0.94200E 00
0.16343E-01	0.22561E-02	0.35700E 00	0.15900E 01	0.15300E 00	0.15300E 00

CORRELATION MATRIX

1.000			
0.550	1.000		
0.739	0.867	1.000	
0.899	0.832	0.859	1.000

2 STEPS

DEPENDENT	INDEPENDENT			
	1	2	3	4
C.298000E-02	0.478000E 00	0.102000E 00	0.525000E 00	
C.385000E-01	0.250500E 01	0.518000E 00	0.497000E 00	
C.450000E-01	0.250000E 01	0.517000E 00	0.485000E 00	
C.206000E-01	0.425000E 00	0.277000E 01	0.310000E 00	
C.185000E-01	0.433000E 00	0.280000E 01	0.270000E 00	
C.180000E-01	0.489000E 00	0.562000E 00	0.510000E-01	
C.103000E-01	0.546000E 00	0.506000E 00	0.446000E 00	
C.121500E-01	0.469000E 00	0.556000E 00	0.475000E 00	
C.705000E-02	0.100000E 00	0.540000E 00	0.464000E 00	
C.824000E-02	0.422000E 00	0.462000E 00	0.261500E 01	
C.734000E-02	0.467000E 00	0.485000E 00	0.255500E 01	
C.315000E-01	0.149500E 01	0.511000E 00	0.495000E 00	
C.435000E-01	0.122200E 01	0.776000E 00	0.103000E 00	

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

Mechanism (d)
 Experimental Data - 275°C
 Non-Linear Regression - Initial parameters from Linear Regression

PHI= 0.10037E-03 PARAMETERS	SQRT(PHI)/ND= 0.77067E-03 0.25000E 00	0.58000E 00	LAMBDA= 0.10000E-01 0.19000E 00	0.88000E 00	MATRIX
PHI= 0.94398E-04 PARAMETERS	SQRT(PHI)/ND= 0.74737E-03 0.25238E 00	0.59086E 00	LAMBDA= 0.10000E 01 0.17750E 00	0.89016E 00	MATRIX
PHI= 0.94340E-04 PARAMETERS	SQRT(PHI)/ND= 0.74714E-03 0.25169E 00	0.59068E 00	LAMBDA= 0.99999E-01 0.17740E 00	0.88991E 00	MATRIX
PHI= 0.94330E-04 PARAMETERS	SQRT(PHI)/ND= 0.74710E-03 0.25165E 00	0.59067E 00	LAMBDA= 0.99999E-01 0.17745E 00	0.88991E 00	MATRIX
PHI= 0.94319E-04 PARAMETERS	SQRT(PHI)/ND= 0.74706E-03 0.25162E 00	0.59067E 00	LAMBDA= 0.99999E-01 0.17750E 00	0.88991E 00	MATRIX
PHI= 0.94310E-04 PARAMETERS	SQRT(PHI)/ND= 0.74702E-03 0.25159E 00	0.59066E 00	LAMBDA= 0.99999E-01 0.17755E 00	0.88991E 00	MATRIX
PHI= 0.94300E-04 PARAMETERS	SQRT(PHI)/ND= 0.74698E-03 0.25156E 00	0.59066E 00	LAMBDA= 0.99999E-01 0.17760E 00	0.88991E 00	MATRIX
PHI= 0.94291E-04 PARAMETERS	SQRT(PHI)/ND= 0.74695E-03 0.25153E 00	0.59065E 00	LAMBDA= 0.99999E-01 0.17764E 00	0.88990E 00	MATRIX
PHI= 0.94282E-04 PARAMETERS	SQRT(PHI)/ND= 0.74691E-03 0.25150E 00	0.59065E 00	LAMBDA= 0.99999E-01 0.17769E 00	0.88990E 00	MATRIX
PHI= 0.94273E-04 PARAMETERS	SQRT(PHI)/ND= 0.74688E-03 0.25148E 00	0.59064E 00	LAMBDA= 0.99999E-01 0.17774E 00	0.88990E 00	MATRIX
PHI= 0.94265E-04 PARAMETERS	SQRT(PHI)/ND= 0.74684E-03 0.25145E 00	0.59063E 00	LAMBDA= 0.99999E-01 0.17779E 00	0.88990E 00	MATRIX
PHI= 0.94257E-04 PARAMETERS	SQRT(PHI)/ND= 0.74681E-03 0.25143E 00	0.59063E 00	LAMBDA= 0.99999E-01 0.17783E 00	0.88990E 00	MATRIX
PHI= 0.94249E-04 PARAMETERS	SQRT(PHI)/ND= 0.74678E-03 0.25141E 00	0.59062E 00	LAMBDA= 0.99999E-01 0.17788E 00	0.88990E 00	MATRIX
PHI= 0.94241E-04 PARAMETERS	SQRT(PHI)/ND= 0.74675E-03 0.25139E 00	0.59061E 00	LAMBDA= 0.99999E-01 0.17793E 00	0.88990E 00	MATRIX
PHI= 0.94233E-04 PARAMETERS	SQRT(PHI)/ND= 0.74672E-03 0.25137E 00	0.59061E 00	LAMBDA= 0.99999E-01 0.17797E 00	0.88990E 00	MATRIX
PHI= 0.94225E-04 PARAMETERS	SQRT(PHI)/ND= 0.74669E-03 0.25135E 00	0.59060E 00	LAMBDA= 0.99999E-01 0.17802E 00	0.88990E 00	MATRIX
PHI= 0.94218E-04 PARAMETERS	SQRT(PHI)/ND= 0.74666E-03 0.25134E 00	0.59059E 00	LAMBDA= 0.99999E-01 0.17807E 00	0.88990E 00	MATRIX
PHI= 0.94211E-04 PARAMETERS	SQRT(PHI)/ND= 0.74663E-03 0.25132E 00	0.59059E 00	LAMBDA= 0.99999E-01 0.17811E 00	0.88990E 00	MATRIX
PHI= 0.94204E-04 PARAMETERS	SQRT(PHI)/ND= 0.74660E-03 0.25131E 00	0.59058E 00	LAMBDA= 0.99999E-01 0.17816E 00	0.88990E 00	MATRIX
PHI= 0.94197E-04	SQRT(PHI)/ND= 0.74657E-03		LAMBDA= 0.99999E-01		MATRIX

PARAMETERS	0.25130E 00	0.59057E 00	0.17820E 00	0.88989E 00	
HI= 0.94190E-04	SQRT(PHI)/ND= 0.74655E-03		LAMBDA= 0.99999E-01		MATRIX
PARAMETERS	0.25128E 00	0.59057E 00	0.17825E 00	0.88989E 00	
HI= 0.94183E-04	SQRT(PHI)/ND= 0.74652E-03		LAMBDA= 0.99999E-01		MATRIX
PARAMETERS	0.25127E 00	0.59056E 00	0.17830E 00	0.88989E 00	
HI= 0.94176E-04	SQRT(PHI)/ND= 0.74649E-03		LAMBDA= 0.99999E-01		MATRIX
PARAMETERS	0.25126E 00	0.59055E 00	0.17834E 00	0.88989E 00	
HI= 0.94170E-04	SQRT(PHI)/ND= 0.74647E-03		LAMBDA= 0.99999E-01		MATRIX
PARAMETERS	0.25125E 00	0.59054E 00	0.17839E 00	0.88989E 00	
HI= 0.94163E-04	SQRT(PHI)/ND= 0.74644E-03		LAMBDA= 0.99999E-01		MATRIX
PARAMETERS	0.25124E 00	0.59053E 00	0.17843E 00	0.88989E 00	
HI= 0.94157E-04	SQRT(PHI)/ND= 0.74642E-03		LAMBDA= 0.99999E-01		MATRIX
PARAMETERS	0.25124E 00	0.59053E 00	0.17848E 00	0.88989E 00	
HI= 0.94150E-04	SQRT(PHI)/ND= 0.74639E-03		LAMBDA= 0.99999E-01		MATRIX
PARAMETERS	0.25123E 00	0.59052E 00	0.17852E 00	0.88989E 00	

ALGORITHM TERMINATED

HI= 0.94150E-04	SQRT(PHI)/ND= 0.74639E-03		LAMBDA= 0.99999E 04		MATRIX
PARAMETERS	0.25123E 00	0.59052E 00	0.17852E 00	0.88989E 00	

DEPENDENT	DIFFERENCE	INDEPENDENT	1	2	3	4
0.39656E-02	-0.98560E-03	0.47800E 00	0.10200E 00	0.52500E 00		
0.41820E-01	-0.29203E-02	0.25050E 01	0.51800E 00	0.49700E 00		
0.41820E-01	0.31790E-02	0.25000E 01	0.51700E 00	0.48500E 00		
0.19854E-01	0.74501E-03	0.42500E 00	0.27700E 01	0.31000E 00		
0.20265E-01	-0.17651E-02	0.43300E 00	0.28000E 01	0.27000E 00		
0.16932E-01	0.10676E-02	0.48900E 00	0.56200E 00	0.51000E-01		
0.15879E-01	-0.55791E-02	0.54600E 00	0.50600E 00	0.44600E 00		
0.14688E-01	-0.25383E-02	0.46900E 00	0.55600E 00	0.47500E 00		
0.35018E-02	0.35481E-02	0.10000E 00	0.54000E 00	0.46400E 00		
0.75559E-02	0.68403E-03	0.42200E 00	0.46200E 00	0.26150E 01		
0.86446E-02	-0.13046E-02	0.46700E 00	0.48500E 00	0.25550E 01		
0.32349E-01	-0.44974E-03	0.14950E 01	0.51100E 00	0.49500E 00		
0.39352E-01	0.41475E-02	0.12220E 01	0.77600E 00	0.10300E 00		

CORRELATION MATRIX

1.000			
0.749	1.000		
0.702	0.788	1.000	
0.944	0.904	0.763	1.000

27 STEPS

DEPENDENT	INDEPENDENT	2	3	4
	1			
0.29800E-02	0.47800E 00	0.10200E 00	0.52500E 00	
0.38900E-01	0.25050E 01	0.51800E 00	0.49700E 00	
0.45000E-01	0.25000E 01	0.51700E 00	0.48500E 00	
0.20600E-01	0.42500E 00	0.27700E 01	0.31000E 00	
0.18500E-01	0.43300E 00	0.28000E 01	0.27000E 00	
0.18000E-01	0.48900E 00	0.56200E 00	0.51000E-01	
0.10300E-01	0.54600E 00	0.50600E 00	0.44600E 00	
0.12150E-01	0.46900E 00	0.55600E 00	0.47500E 00	
0.70500E-02	0.10000E 00	0.54000E 00	0.46400E 00	
0.82400E-02	0.42200E 00	0.46200E 00	0.26150E 01	
0.73400E-02	0.46700E 00	0.48500E 00	0.25550E 01	
0.31900E-01	0.14950E 01	0.51100E 00	0.49500E 00	
0.43500E-01	0.12220E 01	0.77600E 00	0.10300E 00	

Mechanism (d)

Experimental Data - 275°C

Non-Linear Regression - Initial constants from Linear Reg. $\pm 10\%$

PHI= 0.37731E-03 PARAMETERS	SQRT(PHI)/ND= 0.14942E-02 0.28000E 00	0.64000E 00	LAMBDA= 0.10000E-01 0.21000E 00	0.97000E 00	MATRIX
PHI= 0.11278E-03 PARAMETERS	SQRT(PHI)/ND= 0.81692E-03 0.23145E 00	0.58555E 00	LAMBDA= 0.10000E-02 0.15505E 00	0.97318E 00	MATRIX
PHI= 0.11083E-03 PARAMETERS	SQRT(PHI)/ND= 0.80983E-03 0.23038E 00	0.58238E 00	LAMBDA= 0.99999E 01 0.14728E 00	0.97022E 00	MATRIX
PHI= 0.10994E-03 PARAMETERS	SQRT(PHI)/ND= 0.80658E-03 0.22945E 00	0.57955E 00	LAMBDA= 0.99999E 01 0.13985E 00	0.96763E 00	MATRIX
PHI= 0.10985E-03 PARAMETERS	SQRT(PHI)/ND= 0.80622E-03 0.22864E 00	0.57700E 00	LAMBDA= 0.99999E 01 0.13269E 00	0.96536E 00	MATRIX
PHI= 0.10983E-03 PARAMETERS	SQRT(PHI)/ND= 0.80618E-03 0.22854E 00	0.57669E 00	LAMBDA= 0.99999E 02 0.13186E 00	0.96508E 00	MATRIX
PHI= 0.10974E-03 PARAMETERS	SQRT(PHI)/ND= 0.80583E-03 0.22848E 00	0.57666E 00	LAMBDA= 0.99999E 01 0.13184E 00	0.96506E 00	MATRIX
PHI= 0.10891E-03 PARAMETERS	SQRT(PHI)/ND= 0.80279E-03 0.22791E 00	0.57639E 00	LAMBDA= 0.99999E 00 0.13158E 00	0.96482E 00	MATRIX
PHI= 0.10565E-03 PARAMETERS	SQRT(PHI)/ND= 0.79067E-03 0.22483E 00	0.57456E 00	LAMBDA= 0.99999E-01 0.12950E 00	0.96346E 00	MATRIX
PHI= 0.10472E-03 PARAMETERS	SQRT(PHI)/ND= 0.78720E-03 0.22306E 00	0.57318E 00	LAMBDA= 0.99999E-01 0.12763E 00	0.96261E 00	MATRIX
PHI= 0.10463E-03 PARAMETERS	SQRT(PHI)/ND= 0.78685E-03 0.22204E 00	0.57205E 00	LAMBDA= 0.99999E-01 0.12587E 00	0.96205E 00	MATRIX
PHI= 0.10463E-03 PARAMETERS	SQRT(PHI)/ND= 0.78684E-03 0.22191E 00	0.57193E 00	LAMBDA= 0.99999E 00 0.12568E 00	0.96199E 00	MATRIX
PHI= 0.10461E-03 PARAMETERS	SQRT(PHI)/ND= 0.78676E-03 0.22183E 00	0.57192E 00	LAMBDA= 0.99999E-01 0.12568E 00	0.96198E 00	MATRIX
PHI= 0.10449E-03 PARAMETERS	SQRT(PHI)/ND= 0.78631E-03 0.22130E 00	0.57182E 00	LAMBDA= 0.99999E-02 0.12562E 00	0.96194E 00	MATRIX
PHI= 0.10441E-03 PARAMETERS	SQRT(PHI)/ND= 0.78601E-03 0.22050E 00	0.57105E 00	LAMBDA= 0.99999E-03 0.12511E 00	0.96174E 00	MATRIX
PHI= 0.10440E-03 PARAMETERS	SQRT(PHI)/ND= 0.78600E-03 0.22040E 00	0.57097E 00	LAMBDA= 0.99999E-02 0.12506E 00	0.96172E 00	MATRIX
PHI= 0.10440E-03 PARAMETERS	SQRT(PHI)/ND= 0.78600E-03 0.22040E 00	0.57097E 00	LAMBDA= 0.99999E 00 0.12506E 00	0.96172E 00	MATRIX
PHI= 0.10440E-03 PARAMETERS	SQRT(PHI)/ND= 0.78600E-03 0.22040E 00	0.57097E 00	LAMBDA= 0.99999E 00 0.12506E 00	0.96172E 00	MATRIX

ALGORITHM CONVERGED

		1		2		3	
0.39051E-02	-0.92514E-03	0.47800E 00		0.10200E 00		0.52500E 00	
0.43047E-01	-0.41470E-02	0.25050E 01		0.51200E 00		0.49700E 00	
0.43021E-01	0.19789E-02	0.25000E 01		0.51700E 00		0.48500E 00	
0.19343E-01	0.12568E-02	0.42500E 00		0.27700E 01		0.31000E 00	
0.19718E-01	-0.12183E-02	0.43300E 00		0.28000E 01		0.27000E 00	
0.16151E-01	0.18487E-02	0.48900E 00		0.56200E 00		0.51000E-01	
0.15578E-01	-0.52789E-02	0.54600E 00		0.50600E 00		0.44600E 00	
0.14403E-01	-0.22537E-02	0.46900E 00		0.55600E 00		0.47500E 00	
0.33504E-02	0.36595E-02	0.10000E 00		0.54000E 00		0.46400E 00	
0.83223E-02	-0.82321E-04	0.42200E 00		0.46200E 00		0.26150E 01	
0.94921E-02	-0.21521E-02	0.46700E 00		0.48500E 00		0.25550E 01	
0.32635E-01	-0.73558E-03	0.14950E 01		0.51100E 00		0.49500E 00	
0.38556E-01	0.49434E-02	0.12220E 01		0.77600E 00		0.10300E 00	

CORRELATION MATRIX

1.000			
0.781	1.000		
0.701	0.768	1.000	
0.954	0.912	0.744	1.000

17 STEPS

DEPENDENT	INDEPENDENT			
	1	2	3	4
0.29800E-02	0.47800E 00	0.10200E 00	0.52500E 00	
0.38900E-01	0.25050E 01	0.51800E 00	0.49700E 00	
0.45000E-01	0.25000E 01	0.51700E 00	0.48500E 00	
0.20600E-01	0.42500E 00	0.27700E 01	0.31000E 00	
0.18500E-01	0.43300E 00	0.28000E 01	0.27000E 00	
0.18000E-01	0.48900E 00	0.56200E 00	0.51000E-01	
0.10300E-01	0.54600E 00	0.50600E 00	0.44600E 00	
0.12150E-01	0.46900E 00	0.55600E 00	0.47500E 00	
0.70500E-02	0.10000E 00	0.54000E 00	0.46400E 00	
0.82400E-02	0.42200E 00	0.46200E 00	0.26150E 01	
0.73400E-02	0.46700E 00	0.48500E 00	0.25550E 01	
0.31900E-01	0.14950E 01	0.51100E 00	0.49500E 00	
0.43500E-01	0.12220E 01	0.77600E 00	0.10300E 00	

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

Mechanism (d)
 Experimental Data - 275°

Non-linear Regression - Initial parameters from Linear Regression - 10%

PHI= 0.53012E-03 PARAMETERS	SQRT(PHI)/ND= 0.17711E-02 0.22000E 00	0.52000E 00	LAMBDA= 0.10000E-01 0.17000E 00	0.79000E 00	MATRIX
PHI= 0.28105E-03 PARAMETERS	SQRT(PHI)/ND= 0.12895E-02 0.24196E 00	0.61574E 00	LAMBDA= 0.99999E-02 0.46430E-01	0.94477E 00	MATRIX
PHI= 0.26881E-03 PARAMETERS	SQRT(PHI)/ND= 0.12611E-02 0.23399E 00	0.58822E 00	LAMBDA= 0.99999E 00 -0.10322E-01	0.92450E 00	MATRIX
PHI= 0.26800E-03 PARAMETERS	SQRT(PHI)/ND= 0.12592E-02 0.23166E 00	0.58157E 00	LAMBDA= 0.99999E 01 -0.22228E-01	0.91883E 00	MATRIX
PHI= 0.26799E-03 PARAMETERS	SQRT(PHI)/ND= 0.12592E-02 0.23163E 00	0.58149E 00	LAMBDA= 0.99999E 03 -0.22365E-01	0.91876E 00	MATRIX
PHI= 0.26798E-03 PARAMETERS	SQRT(PHI)/ND= 0.12592E-02 0.23161E 00	0.58141E 00	LAMBDA= 0.99999E 03 -0.22501E-01	0.91869E 00	MATRIX
PHI= 0.26793E-03 PARAMETERS	SQRT(PHI)/ND= 0.12591E-02 0.23159E 00	0.58141E 00	LAMBDA= 0.99999E 02 -0.22513E-01	0.91868E 00	MATRIX
PHI= 0.26734E-03 PARAMETERS	SQRT(PHI)/ND= 0.12577E-02 0.23141E 00	0.58133E 00	LAMBDA= 0.99999E 01 -0.22633E-01	0.91861E 00	MATRIX
PHI= 0.26235E-03 PARAMETERS	SQRT(PHI)/ND= 0.12459E-02 0.22977E 00	0.58061E 00	LAMBDA= 0.99999E 00 -0.23791E-01	0.91791E 00	MATRIX
PHI= 0.24956E-03 PARAMETERS	SQRT(PHI)/ND= 0.12152E-02 0.22134E 00	0.57619E 00	LAMBDA= 0.99999E-01 -0.33052E-01	0.91427E 00	MATRIX
PHI= 0.24860E-03 PARAMETERS	SQRT(PHI)/ND= 0.12128E-02 0.22029E 00	0.57568E 00	LAMBDA= 0.99999E 00 -0.34122E-01	0.91384E 00	MATRIX
PHI= 0.24796E-03 PARAMETERS	SQRT(PHI)/ND= 0.12113E-02 0.21929E 00	0.57520E 00	LAMBDA= 0.99999E 00 -0.35182E-01	0.91344E 00	MATRIX
PHI= 0.24761E-03 PARAMETERS	SQRT(PHI)/ND= 0.12104E-02 0.21836E 00	0.57474E 00	LAMBDA= 0.99999E 00 -0.36235E-01	0.91306E 00	MATRIX
PHI= 0.24750E-03 PARAMETERS	SQRT(PHI)/ND= 0.12101E-02 0.21747E 00	0.57430E 00	LAMBDA= 0.99999E 00 -0.37281E-01	0.91271E 00	MATRIX
PHI= 0.24749E-03 PARAMETERS	SQRT(PHI)/ND= 0.12101E-02 0.21738E 00	0.57425E 00	LAMBDA= 0.99999E 01 -0.37387E-01	0.91267E 00	MATRIX
PHI= 0.24749E-03 PARAMETERS	SQRT(PHI)/ND= 0.12101E-02 0.21729E 00	0.57421E 00	LAMBDA= 0.99999E 01 -0.37494E-01	0.91264E 00	MATRIX
PHI= 0.24749E-03 PARAMETERS	SQRT(PHI)/ND= 0.12101E-02 0.21720E 00	0.57416E 00	LAMBDA= 0.99999E 01 -0.37600E-01	0.91260E 00	MATRIX
PHI= 0.24749E-03 PARAMETERS	SQRT(PHI)/ND= 0.12101E-02 0.21719E 00	0.57416E 00	LAMBDA= 0.99999E 02 -0.37611E-01	0.91260E 00	MATRIX
PHI= 0.24748E-03 PARAMETERS	SQRT(PHI)/ND= 0.12101E-02 0.21719E 00	0.57416E 00	LAMBDA= 0.99999E 01 -0.37612E-01	0.91260E 00	MATRIX
PHI= 0.24738E-03	SQRT(PHI)/ND= 0.12098E-02		LAMBDA= 0.99999E 00		MATRIX

PARAMETERS	0.21713E 00	0.57415E 00	-0.37621E-01	0.91259E 00	
PHI= 0.24651E-03	SQRT(PHI)/ND= 0.12077E-02		LAMBDA= 0.99999E-01		MATRIX
PARAMETERS	0.21655E 00	0.57412E 00	-0.37718E-01	0.91256E 00	
PHI= 0.24226E-03	SQRT(PHI)/ND= 0.11972E-02		LAMBDA= 0.99999E-02		MATRIX
PARAMETERS	0.21268E 00	0.57380E 00	-0.38613E-01	0.91232E 00	
PHI= 0.24079E-03	SQRT(PHI)/ND= 0.11936E-02		LAMBDA= 0.99999E-02		MATRIX
PARAMETERS	0.20993E 00	0.57354E 00	-0.39453E-01	0.91216E 00	
PHI= 0.24072E-03	SQRT(PHI)/ND= 0.11934E-02		LAMBDA= 0.99999E-02		MATRIX
PARAMETERS	0.20800E 00	0.57332E 00	-0.40259E-01	0.91204E 00	
PHI= 0.24072E-03	SQRT(PHI)/ND= 0.11934E-02		LAMBDA= 0.99999E 03		MATRIX
PARAMETERS	0.20800E 00	0.57332E 00	-0.40259E-01	0.91204E 00	
PHI= 0.24072E-03	SQRT(PHI)/ND= 0.11934E-02		LAMBDA= 0.99999E 03		MATRIX
PARAMETERS	0.20800E 00	0.57332E 00	-0.40259E-01	0.91204E 00	

ALGORITHM CONVERGED

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3	4
		1			
0.41037E-02	-0.11237E-02	0.47800E 00	0.10200E 00	0.52500E 00	
0.43655E-01	-0.47553E-02	0.25050E 01	0.51800E 00	0.49700E 00	
0.43538E-01	0.14611E-02	0.25000E 01	0.51700E 00	0.48500E 00	
0.18041E-01	0.25580E-02	0.42500E 00	0.27700E 01	0.31000E 00	
0.18298E-01	0.20167E-03	0.43300E 00	0.28000E 01	0.27000E 00	
0.14784E-01	0.32150E-02	0.48900E 00	0.56200E 00	0.51000E-01	
0.15649E-01	-0.53490E-02	0.54600E 00	0.50600E 00	0.44600E 00	
0.14528E-01	-0.23786E-02	0.46900E 00	0.55600E 00	0.47500E 00	
0.34135E-02	0.36364E-02	0.10000E 00	0.54000E 00	0.46400E 00	
0.13628E-01	-0.53886E-02	0.42200E 00	0.46200E 00	0.26150E 01	
0.15217E-01	-0.78776E-02	0.46700E 00	0.48500E 00	0.25550E 01	
0.33116E-01	-0.12161E-02	0.14950E 01	0.51100E 00	0.49500E 00	
0.35902E-01	0.75979E-02	0.12220E 01	0.77600E 00	0.10300E 00	

CORRELATION MATRIX

1.000			
0.792	1.000		
0.626	0.608	1.000	
0.953	0.919	0.609	1.000

25 STEPS

DEPENDENT	INDEPENDENT		
	1	2	3
0.29800E-02	0.47800E 00	0.10200E 00	0.52500E 00
0.38900E-01	0.25050E 01	0.51800E 00	0.49700E 00
0.45000E-01	0.25000E 01	0.51700E 00	0.48500E 00
0.20600E-01	0.42500E 00	0.27700E 01	0.31000E 00
0.18500E-01	0.43300E 00	0.28000E 01	0.27000E 00
0.18000E-01	0.48900E 00	0.56200E 00	0.51000E-01
0.10300E-01	0.54600E 00	0.50600E 00	0.44600E 00
0.12150E-01	0.46900E 00	0.55600E 00	0.47500E 00
0.70500E-02	0.10000E 00	0.54000E 00	0.46400E 00
0.82400E-02	0.42200E 00	0.46200E 00	0.26150E 01
0.73400E-02	0.46700E 00	0.48500E 00	0.25550E 01
0.31900E-01	0.14950E 01	0.51100E 00	0.49500E 00
0.43500E-01	0.12220E 01	0.77600E 00	0.10300E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.10799E-03 Sqrt(PHI)/ND= 0.79937E-03 LAMBDA= 0.10000E-01 MATRIX
 PARAMETERS 0.26000E 00 0.57000E 00 0.13000E 00 0.87000E 00

PHI= 0.10419E-03 Sqrt(PHI)/ND= 0.78521E-03 LAMBDA= 0.99999E-02 MATRIX
 PARAMETERS 0.26000E 00 0.56999E 00 0.16445E 00 0.86662E 00

PHI= 0.10347E-03 Sqrt(PHI)/ND= 0.78249E-03 LAMBDA= 0.99999E 00 MATRIX
 PARAMETERS 0.26042E 00 0.58210E 00 0.14569E 00 0.87535E 00

ALGORITHM TERMINATED

PHI= 0.10347E-03 Sqrt(PHI)/ND= 0.78249E-03 LAMBDA= 0.10000E 04 MATRIX
 PARAMETERS 0.26042E 00 0.58210E 00 0.14569E 00 0.87535E 00

SINGULAR MATRIX

DEPENDENT	DIFFERENCE	INDEPENDENT		
		1	2	3
0.40730E-02	-0.10930E-02	0.47800E 00	0.10200E 00	0.52500E 00
0.41936E-01	-0.30369E-02	0.25050E 01	0.51800E 00	0.49700E 00
0.41922E-01	0.30773E-02	0.25000E 01	0.51700E 00	0.48500E 00
0.20385E-01	0.21458E-03	0.42500E 00	0.27700E 01	0.31000E 00
0.20787E-01	-0.22875E-02	0.43300E 00	0.28000E 01	0.27000E 00
0.17063E-01	0.93652E-03	0.48900E 00	0.56200E 00	0.51000E-01
0.16256E-01	-0.59568E-02	0.54600E 00	0.50600E 00	0.44600E 00
0.15076E-01	-0.29262E-02	0.46900E 00	0.55600E 00	0.47500E 00
0.36146E-02	0.34353E-02	0.10000E 00	0.54000E 00	0.46400E 00
0.83537E-02	-0.11373E-03	0.42200E 00	0.46200E 00	0.26150E 01
0.95267E-02	-0.21867E-02	0.46700E 00	0.48500E 00	0.25550E 01
0.32767E-01	-0.86753E-03	0.14950E 01	0.51100E 00	0.49500E 00
0.39495E-01	0.40046E-02	0.12220E 01	0.77600E 00	0.10300E 00

CORRELATION MATRIX

1.000			
0.736	1.000		
0.681	0.759	1.000	
0.937	0.903	0.736	1.000

3 STEPS

DEPENDENT	INDEPENDENT 1	2	3
0.29800E-02	0.47800E 00	0.10200E 00	0.52500E 00
0.38900E-01	0.25050E 01	0.51800E 00	0.49700E 00
0.45000E-01	0.25000E 01	0.51700E 00	0.48500E 00
0.20600E-01	0.42500E 00	0.27700E 01	0.31000E 00
0.18500E-01	0.43300E 00	0.28000E 01	0.27000E 00
0.18000E-01	0.48900E 00	0.56200E 00	0.51000E-01
0.10300E-01	0.54600E 00	0.50600E 00	0.44600E 00
0.12150E-01	0.46900E 00	0.55600E 00	0.47500E 00
0.70500E-02	0.10000E 00	0.54000E 00	0.46400E 00
0.82400E-02	0.42200E 00	0.46200E 00	0.26150E 01
0.73400E-02	0.46700E 00	0.48500E 00	0.25550E 01
0.31900E-01	0.14950E 01	0.51100E 00	0.49500E 00
0.43500E-01	0.12220E 01	0.77600E 00	0.10300E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.13904E-03 PARAMETERS	SQRT(PHI)/ND= 0.90705E-03 0.26000E 00	0.52000E 00	LAMBDA= 0.10000E-01 0.13000E 00	0.87000E 00	MATRI
PHI= 0.11637E-03 PARAMETERS	SQRT(PHI)/ND= 0.82983E-03 0.26129E 00	0.54310E 00	LAMBDA= 0.10000E 01 0.11293E 00	0.88625E 00	MATRI
PHI= 0.10466E-03 PARAMETERS	SQRT(PHI)/ND= 0.78696E-03 0.26129E 00	0.54310E 00	LAMBDA= 0.99999E-02 0.16093E 00	0.90440E 00	MATRI
PHI= 0.10459E-03 PARAMETERS	SQRT(PHI)/ND= 0.78672E-03 0.26089E 00	0.54439E 00	LAMBDA= 0.99999E 01 0.15824E 00	0.90481E 00	MATRI
PHI= 0.10272E-03 PARAMETERS	SQRT(PHI)/ND= 0.77964E-03 0.26090E 00	0.54439E 00	LAMBDA= 0.99999E-02 0.21776E 00	0.90647E 00	MATRI
PHI= 0.94225E-04 PARAMETERS	SQRT(PHI)/ND= 0.74669E-03 0.25911E 00	0.55967E 00	LAMBDA= 0.99999E 00 0.21346E 00	0.91365E 00	MATRI
PHI= 0.93282E-04 PARAMETERS	SQRT(PHI)/ND= 0.74294E-03 0.25637E 00	0.56903E 00	LAMBDA= 0.99999E 00 0.20155E 00	0.91645E 00	MATRI
PHI= 0.92292E-04 PARAMETERS	SQRT(PHI)/ND= 0.73899E-03 0.25393E 00	0.56835E 00	LAMBDA= 0.99999E-01 0.20123E 00	0.91558E 00	MATRI
PHI= 0.92100E-04 PARAMETERS	SQRT(PHI)/ND= 0.73822E-03 0.25268E 00	0.56800E 00	LAMBDA= 0.99999E-01 0.20107E 00	0.91514E 00	MATRI
PHI= 0.92099E-04 PARAMETERS	SQRT(PHI)/ND= 0.73821E-03 0.25266E 00	0.56808E 00	LAMBDA= 0.99999E 02 0.20088E 00	0.91518E 00	MATRI
PHI= 0.92099E-04 PARAMETERS	SQRT(PHI)/ND= 0.73821E-03 0.25264E 00	0.56816E 00	LAMBDA= 0.99999E 02 0.20069E 00	0.91521E 00	MATRI
PHI= 0.92076E-04 PARAMETERS	SQRT(PHI)/ND= 0.73812E-03 0.25196E 00	0.56797E 00	LAMBDA= 0.99999E-01 0.20060E 00	0.91497E 00	MATRI
PHI= 0.92027E-04 PARAMETERS	SQRT(PHI)/ND= 0.73793E-03 0.25186E 00	0.56889E 00	LAMBDA= 0.99999E 01 0.19887E 00	0.91545E 00	MATRI
PHI= 0.92012E-04 PARAMETERS	SQRT(PHI)/ND= 0.73787E-03 0.25123E 00	0.56872E 00	LAMBDA= 0.99999E-01 0.19879E 00	0.91523E 00	MATRI
PHI= 0.91998E-04 PARAMETERS	SQRT(PHI)/ND= 0.73781E-03 0.25114E 00	0.56959E 00	LAMBDA= 0.99999E 01 0.19698E 00	0.91571E 00	MATRI
PHI= 0.91985E-04 PARAMETERS	SQRT(PHI)/ND= 0.73776E-03 0.25055E 00	0.56942E 00	LAMBDA= 0.99999E-01 0.19690E 00	0.91550E 00	MATRI
PHI= 0.91984E-04 PARAMETERS	SQRT(PHI)/ND= 0.73775E-03 0.25055E 00	0.56951E 00	LAMBDA= 0.99999E 02 0.19671E 00	0.91555E 00	MATRI
PHI= 0.89578E-04 PARAMETERS	SQRT(PHI)/ND= 0.72804E-03 0.25055E 00	0.56938E 00	LAMBDA= 0.99999E 02 0.22938E 00	0.92303E 00	MATRI
PHI= 0.89133E-04 PARAMETERS	SQRT(PHI)/ND= 0.72623E-03 0.25059E 00	0.57066E 00	LAMBDA= 0.99999E 01 0.22902E 00	0.92385E 00	MATRI
PHI= 0.88635E-04	SQRT(PHI)/ND= 0.72420E-03		LAMBDA= 0.99999E 00		MATRI

PARAMETERS	0.24951E 00	0.57809E 00	0.21945E 00	0.92738E 00	
PHI= 0.88207E-04	SQRT(PHI)/ND= 0.72245E-03	LAMBDA= 0.99999E-01			MATRI
PARAMETERS	0.24788E 00	0.57765E 00	0.21925E 00	0.92682E 00	
PHI= 0.88135E-04	SQRT(PHI)/ND= 0.72215E-03	LAMBDA= 0.99999E-01			MATRI
PARAMETERS	0.24709E 00	0.57744E 00	0.21915E 00	0.92655E 00	
PHI= 0.88132E-04	SQRT(PHI)/ND= 0.72214E-03	LAMBDA= 0.99999E-01			MATRI
PARAMETERS	0.24670E 00	0.57734E 00	0.21910E 00	0.92641E 00	
PHI= 0.88132E-04	SQRT(PHI)/ND= 0.72214E-03	LAMBDA= 0.99999E 03			MATRI
PARAMETERS	0.24670E 00	0.57734E 00	0.21908E 00	0.92642E 00	
PHI= 0.86687E-04	SQRT(PHI)/ND= 0.71619E-03	LAMBDA= 0.99999E 02			MATRI
PARAMETERS	0.24671E 00	0.57724E 00	0.24337E 00	0.93195E 00	
PHI= 0.86438E-04	SQRT(PHI)/ND= 0.71517E-03	LAMBDA= 0.99999E 01			MATRI
PARAMETERS	0.24675E 00	0.57821E 00	0.24295E 00	0.93259E 00	
PHI= 0.86283E-04	SQRT(PHI)/ND= 0.71453E-03	LAMBDA= 0.99999E 01			MATRI
PARAMETERS	0.24674E 00	0.57903E 00	0.24229E 00	0.93310E 00	
PHI= 0.86197E-04	SQRT(PHI)/ND= 0.71417E-03	LAMBDA= 0.99999E 01			MATRI
PARAMETERS	0.24670E 00	0.57974E 00	0.24142E 00	0.93350E 00	
PHI= 0.86161E-04	SQRT(PHI)/ND= 0.71402E-03	LAMBDA= 0.99999E 01			MATRI
PARAMETERS	0.24661E 00	0.58035E 00	0.24036E 00	0.93381E 00	
PHI= 0.86161E-04	SQRT(PHI)/ND= 0.71402E-03	LAMBDA= 0.99999E 02			MATRI
PARAMETERS	0.24660E 00	0.58040E 00	0.24023E 00	0.93383E 00	
PHI= 0.86160E-04	SQRT(PHI)/ND= 0.71402E-03	LAMBDA= 0.99999E 01			MATRI
PARAMETERS	0.24660E 00	0.58041E 00	0.24023E 00	0.93383E 00	
PHI= 0.86151E-04	SQRT(PHI)/ND= 0.71398E-03	LAMBDA= 0.99999E 00			MATRI
PARAMETERS	0.24654E 00	0.58045E 00	0.24020E 00	0.93385E 00	
PHI= 0.86068E-04	SQRT(PHI)/ND= 0.71363E-03	LAMBDA= 0.99999E-01			MATRI
PARAMETERS	0.24611E 00	0.58092E 00	0.23996E 00	0.93409E 00	
PHI= 0.85663E-04	SQRT(PHI)/ND= 0.71195E-03	LAMBDA= 0.99999E-02			MATRI
PARAMETERS	0.24380E 00	0.58465E 00	0.23745E 00	0.93654E 00	
PHI= 0.85601E-04	SQRT(PHI)/ND= 0.71170E-03	LAMBDA= 0.99999E-02			MATRI
PARAMETERS	0.24193E 00	0.58704E 00	0.23446E 00	0.93849E 00	
PHI= 0.85587E-04	SQRT(PHI)/ND= 0.71164E-03	LAMBDA= 0.99999E-01			MATRI
PARAMETERS	0.24152E 00	0.58713E 00	0.23408E 00	0.93857E 00	
PHI= 0.85572E-04	SQRT(PHI)/ND= 0.71157E-03	LAMBDA= 0.99999E-02			MATRI
PARAMETERS	0.24133E 00	0.58714E 00	0.23407E 00	0.93857E 00	
PHI= 0.85539E-04	SQRT(PHI)/ND= 0.71144E-03	LAMBDA= 0.99999E-03			MATRI
PARAMETERS	0.24073E 00	0.58729E 00	0.23399E 00	0.93874E 00	
PHI= 0.85481E-04	SQRT(PHI)/ND= 0.71120E-03	LAMBDA= 0.99999E-04			MATRI
PARAMETERS	0.23961E 00	0.58844E 00	0.23327E 00	0.94044E 00	
PHI= 0.85475E-04	SQRT(PHI)/ND= 0.71117E-03	LAMBDA= 0.99999E-04			MATRI
PARAMETERS	0.23873E 00	0.58913E 00	0.23249E 00	0.94190E 00	
PHI= 0.85474E-04	SQRT(PHI)/ND= 0.71117E-03	LAMBDA= 0.99999E-03			MATRI
PARAMETERS	0.23851E 00	0.58918E 00	0.23241E 00	0.94203E 00	
PHI= 0.85474E-04	SQRT(PHI)/ND= 0.71117E-03	LAMBDA= 0.99999E-02			MATR
PARAMETERS	0.23849E 00	0.58918E 00	0.23240E 00	0.94204E 00	
PHI= 0.85474E-04	SQRT(PHI)/ND= 0.71117E-03	LAMBDA= 0.99999E 00			MATR
PARAMETERS	0.23848E 00	0.58918E 00	0.23240E 00	0.94204E 00	
PHI= 0.85474E-04	SQRT(PHI)/ND= 0.71117E-03	LAMBDA= 0.99999E 00			MATR
PARAMETERS	0.23848E 00	0.58918E 00	0.23240E 00	0.94204E 00	

ALGORITHM CONVERGED

DEPENDENT	DIFFERENCE	INDEPENDENT		
		1	2	3

C.38418E-02	-0.86183E-03	0.47800E 00	0.10200E 00	0.52500E 00
0.42173E-01	-0.32732E-02	0.25050E 01	0.51800E 00	0.49700E 00
0.42198E-01	0.28012E-02	0.25000E 01	0.51700E 00	0.48500E 00
0.19799E-01	0.80037E-03	0.42500E 00	0.27700E 01	0.31000E 00
C.20242E-01	-0.17420E-02	0.43300E 00	0.28000E 01	0.27000E 00
0.17075E-01	-0.92452E-03	0.48900E 00	0.56200E 00	0.51000E-01
C.15581E-01	-0.52819E-02	0.54600E 00	0.50600E 00	0.44600E 00
0.14370E-01	-0.22204E-02	0.46900E 00	0.55600E 00	0.47500E 00
0.34005E-02	0.36494E-02	0.10000E 00	0.54000E 00	0.46400E 00
0.65789E-02	0.16610E-02	0.42200E 00	0.46200E 00	0.26150E 01
0.75638E-02	-0.22380E-03	0.46700E 00	0.48500E 00	0.25550E 01
0.32181E-01	-0.28149E-03	0.14950E 01	0.51100E 00	0.49500E 00
0.39949E-01	0.35502E-02	0.12220E 01	0.77600E 00	0.10300E 00

CORRELATION MATRIX

1.000			
0.766	1.000		
0.730	0.826	1.000	
0.952	0.906	0.799	1.000

43 STEPS

DEPENDENT

INDEPENDENT

2

3

4

0.20100E-01	0.50000E 00	0.27350E 01	0.27000E 00
0.11400E-01	0.48200E 00	0.56000E 00	0.62000E-01
0.13400E-01	0.50100E 00	0.53300E 00	0.46600E 00
0.94600E-02	0.47500E 00	0.55300E 00	0.47100E 00
0.87100E-02	0.47600E 00	0.55600E 00	0.47800E 00
0.25000E-02	0.10100E 00	0.54800E 00	0.45100E 00
0.33800E-01	0.23350E 01	0.55000E 00	0.61000E 00
0.28600E-01	0.25400E 01	0.45200E 00	0.51000E 00
0.29700E-01	0.24050E 01	0.52400E 00	0.57200E 00
0.44000E-02	0.48900E 00	0.98000E-01	0.51300E 00
0.11060E-01	0.48000E 00	0.48000E 00	0.25500E 01
0.53300E-02	0.55500E 00	0.29900E 00	0.16450E 01
0.18850E-01	0.59900E 00	0.99600E 00	0.90700E 00
0.14140E-01	0.43800E 00	0.15230E 01	0.13600E 00
0.15900E-01	0.47800E 00	0.14800E 01	0.14400E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

Mechanism(d)
 Experimental Data - 325°C
 NON-LINEAR REGRESSION - Initial Parameters from Linear Regr

PHI= 0.95127E-04 PARAMETERS	SQRT(PHI)/ND= 0.65022E-03 0.20000E 00	0.48000E 00	LAMBDA= 0.10000E-01 0.30000E-01	0.89000E 00	MATRIX
PHI= 0.65964E-04 PARAMETERS	SQRT(PHI)/ND= 0.54145E-03 0.18891E 00	0.41364E 00	LAMBDA= 0.99999E-02 0.78758E-01	0.87458E 00	MATRIX
PHI= 0.63085E-04 PARAMETERS	SQRT(PHI)/ND= 0.52950E-03 0.19022E 00	0.41692E 00	LAMBDA= 0.99999E 01 0.87845E-01	0.87893E 00	MATRIX
PHI= 0.61475E-04 PARAMETERS	SQRT(PHI)/ND= 0.52270E-03 0.19136E 00	0.41984E 00	LAMBDA= 0.99999E 01 0.96555E-01	0.88269E 00	MATRIX
PHI= 0.60764E-04 PARAMETERS	SQRT(PHI)/ND= 0.51967E-03 0.19234E 00	0.42247E 00	LAMBDA= 0.99999E 01 0.10498E 00	0.88598E 00	MATRIX
PHI= 0.60701E-04 PARAMETERS	SQRT(PHI)/ND= 0.51940E-03 0.19319E 00	0.42488E 00	LAMBDA= 0.99999E 01 0.11319E 00	0.88887E 00	MATRIX
PHI= 0.59963E-04 PARAMETERS	SQRT(PHI)/ND= 0.51624E-03 0.19372E 00	0.42517E 00	LAMBDA= 0.99999E 00 0.11341E 00	0.88906E 00	MATRIX
PHI= 0.56575E-04 PARAMETERS	SQRT(PHI)/ND= 0.50144E-03 0.19679E 00	0.42723E 00	LAMBDA= 0.99999E-01 0.11518E 00	0.89025E 00	MATRIX
PHI= 0.55310E-04 PARAMETERS	SQRT(PHI)/ND= 0.49580E-03 0.19864E 00	0.42884E 00	LAMBDA= 0.99999E-01 0.11676E 00	0.89107E 00	MATRIX
PHI= 0.54889E-04 PARAMETERS	SQRT(PHI)/ND= 0.49391E-03 0.19974E 00	0.43016E 00	LAMBDA= 0.99999E-01 0.11823E 00	0.89164E 00	MATRIX
PHI= 0.54811E-04 PARAMETERS	SQRT(PHI)/ND= 0.49356E-03 0.20038E 00	0.43130E 00	LAMBDA= 0.99999E-01 0.11962E 00	0.89205E 00	MATRIX
PHI= 0.54805E-04 PARAMETERS	SQRT(PHI)/ND= 0.49353E-03 0.20046E 00	0.43142E 00	LAMBDA= 0.99999E 00 0.11976E 00	0.89210E 00	MATRIX
PHI= 0.54802E-04 PARAMETERS	SQRT(PHI)/ND= 0.49352E-03 0.20053E 00	0.43154E 00	LAMBDA= 0.99999E 00 0.11991E 00	0.89214E 00	MATRIX
PHI= 0.54801E-04 PARAMETERS	SQRT(PHI)/ND= 0.49351E-03 0.20060E 00	0.43166E 00	LAMBDA= 0.99999E 00 0.12005E 00	0.89218E 00	MATRIX
PHI= 0.54801E-04 PARAMETERS	SQRT(PHI)/ND= 0.49351E-03 0.20061E 00	0.43167E 00	LAMBDA= 0.99999E 01 0.12006E 00	0.89219E 00	MATRIX
PHI= 0.54800E-04 PARAMETERS	SQRT(PHI)/ND= 0.49351E-03 0.20061E 00	0.43168E 00	LAMBDA= 0.99999E 01 0.12008E 00	0.89219E 00	MATRIX
PHI= 0.54800E-04 PARAMETERS	SQRT(PHI)/ND= 0.49351E-03 0.20062E 00	0.43169E 00	LAMBDA= 0.99999E 01 0.12009E 00	0.89220E 00	MATRIX
PHI= 0.54800E-04 PARAMETERS	SQRT(PHI)/ND= 0.49351E-03 0.20062E 00	0.43169E 00	LAMBDA= 0.99999E 03 0.12009E 00	0.89220E 00	MATRIX
PHI= 0.53471E-04 PARAMETERS	SQRT(PHI)/ND= 0.48749E-03 0.20063E 00	0.44522E 00	LAMBDA= 0.99999E-02 0.12009E 00	0.89227E 00	MATRIX

PHI= 0.53010E-04 PARAMETERS	SQRT(PHI)/ND= 0.48539E-03 0.19822E 00 0.44543E 00	LAMBDA= 0.99999E-03 0.12035E 00 0.89219E 00	MATR
PHI= 0.53001E-04 PARAMETERS	SQRT(PHI)/ND= 0.48534E-03 0.19804E 00 0.44545E 00	LAMBDA= 0.99999E-02 0.12037E 00 0.89219E 00	MATR
PHI= 0.52997E-04 PARAMETERS	SQRT(PHI)/ND= 0.48532E-03 0.19790E 00 0.44548E 00	LAMBDA= 0.99999E-02 0.12040E 00 0.89218E 00	MATR
PHI= 0.52995E-04 PARAMETERS	SQRT(PHI)/ND= 0.48532E-03 0.19779E 00 0.44551E 00	LAMBDA= 0.99999E-02 0.12043E 00 0.89218E 00	MATR
PHI= 0.52995E-04 PARAMETERS	SQRT(PHI)/ND= 0.48532E-03 0.19778E 00 0.44551E 00	LAMBDA= 0.99999E-01 0.12043E 00 0.89218E 00	MATR
PHI= 0.52995E-04 PARAMETERS	SQRT(PHI)/ND= 0.48532E-03 0.19777E 00 0.44552E 00	LAMBDA= 0.99999E-01 0.12043E 00 0.89218E 00	MATR
PHI= 0.52995E-04 PARAMETERS	SQRT(PHI)/ND= 0.48532E-03 0.19776E 00 0.44552E 00	LAMBDA= 0.99999E-01 0.12043E 00 0.89218E 00	MATR
PHI= 0.52897E-04 PARAMETERS	SQRT(PHI)/ND= 0.48487E-03 0.19776E 00 0.44905E 00	LAMBDA= 0.99999E-02 0.12043E 00 0.89215E 00	MATR
PHI= 0.52828E-04 PARAMETERS	SQRT(PHI)/ND= 0.48455E-03 0.19659E 00 0.44919E 00	LAMBDA= 0.99999E-03 0.12069E 00 0.89209E 00	MATR
PHI= 0.52828E-04 PARAMETERS	SQRT(PHI)/ND= 0.48455E-03 0.19659E 00 0.44919E 00	LAMBDA= 0.99999E 00 0.12069E 00 0.89209E 00	MATR
PHI= 0.52828E-04 PARAMETERS	SQRT(PHI)/ND= 0.48455E-03 0.19658E 00 0.44919E 00	LAMBDA= 0.99999E 00 0.12069E 00 0.89209E 00	MATR

ALGORITHM CONVERGED

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3
		1		
0.19351E-01	0.74827E-03	0.50000E 00	0.27350E 01	0.27000E 00
0.11602E-01	-0.20224E-03	0.48200E 00	0.56000E 00	0.62000E-01
0.10823E-01	-0.25769E-02	0.50100E 00	0.53300E 00	0.46600E 00
0.10578E-01	-0.11184E-02	0.47500E 00	0.55300E 00	0.47100E 00
0.10621E-01	-0.19118E-02	0.47600E 00	0.55600E 00	0.47800E 00
0.25007E-02	-0.74133E-06	0.10100E 00	0.54800E 00	0.45100E 00
0.31941E-01	-0.18583E-02	0.23350E 01	0.55000E 00	0.61000E 00
0.29068E-01	-0.46833E-03	0.25400E 01	0.45200E 00	0.51000E 00
0.31432E-01	-0.17323E-02	0.24050E 01	0.52400E 00	0.57200E 00
0.26126E-02	0.17873E-02	0.48900E 00	0.98000E-01	0.51300E 00
0.69354E-02	0.41245E-02	0.48000E 00	0.48000E 00	0.25500E 01
0.62873E-02	-0.95739E-03	0.55500E 00	0.29900E 00	0.16450E 01
0.16759E-01	0.20905E-02	0.59900E 00	0.99600E 00	0.90700E 00
0.16462E-01	-0.23228E-02	0.43800E 00	0.15230E 01	0.13600E 00
0.17665E-01	-0.17658E-02	0.47800E 00	0.14800E 01	0.14400E 00

CORRELATION MATRIX

1.000			
0.776	1.000		
0.771	0.869	1.000	
0.949	0.920	0.839	1.000

29 STEPS

DEPENDENT

INDEPENDENT

	1	2	3	4
0.20100E-01	0.50000E 00	0.27350E 01	0.27000E 00	
0.11400E-01	0.48200E 00	0.56000E 00	0.62000E-01	
0.13400E-01	0.50100E 00	0.53300E 00	0.46600E 00	
0.94600E-02	0.47500E 00	0.55300E 00	0.47100E 00	
0.87100E-02	0.47600E 00	0.55600E 00	0.47800E 00	
0.25000E-02	0.10100E 00	0.54800E 00	0.45100E 00	
0.33800E-01	0.23350E 01	0.55000E 00	0.61000E 00	
0.28600E-01	0.25400E 01	0.45200E 00	0.51000E 00	
0.29700E-01	0.24050E 01	0.52400E 00	0.57200E 00	
0.44000E-02	0.48900E 00	0.98000E-01	0.51300E 00	
0.11060E-01	0.48000E 00	0.48000E 00	0.25500E 01	
0.53300E-02	0.55500E 00	0.29900E 00	0.16450E 01	
0.18850E-01	0.59900E 00	0.99600E 00	0.90700E 00	
0.14140E-01	0.43800E 00	0.15230E 01	0.13600E 00	
0.15900E-01	0.47800E 00	0.14800E 01	0.14400E 00	

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.54918E-04 PARAMETERS	SQRT(PHI)/ND= 0.49404E-03 0.19000E 00	0.45000E 00	LAMBDA= 0.10000E-01 0.12000E 00	0.89000E 00	MATRIX
PHI= 0.53139E-04 PARAMETERS	SQRT(PHI)/ND= 0.48597E-03 0.19315E 00	0.45085E 00	LAMBDA= 0.99999E-01 0.12042E 00	0.89081E 00	MATRIX
PHI= 0.52808E-04 PARAMETERS	SQRT(PHI)/ND= 0.48446E-03 0.19454E 00	0.45123E 00	LAMBDA= 0.99999E-01 0.12061E 00	0.89117E 00	MATRIX
PHI= 0.52749E-04 PARAMETERS	SQRT(PHI)/ND= 0.48419E-03 0.19517E 00	0.45140E 00	LAMBDA= 0.99999E-01 0.12070E 00	0.89134E 00	MATRIX
PHI= 0.52740E-04 PARAMETERS	SQRT(PHI)/ND= 0.48415E-03 0.19545E 00	0.45148E 00	LAMBDA= 0.99999E-01 0.12073E 00	0.89141E 00	MATRIX
PHI= 0.52740E-04 PARAMETERS	SQRT(PHI)/ND= 0.48415E-03 0.19558E 00	0.45151E 00	LAMBDA= 0.99999E-01 0.12075E 00	0.89144E 00	MATRIX

ALGORITHM TERMINATED

PHI= 0.52740E-04 PARAMETERS	SQRT(PHI)/ND= 0.48415E-03 0.19558E 00	0.45151E 00	LAMBDA= 0.10000E 04 0.12075E 00	0.89144E 00	MATRIX
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SINGULAR MATRIX

DEPENDENT

DIFFERENCE

INDEPENDENT

		1	2	3	4
0.19242E-01	0.85733E-03	0.50000E 00	0.27350E 01	0.27000E 00	
0.11580E-01	-0.18020E-03	0.48200E 00	0.56000E 00	0.62000E-01	
0.10803E-01	0.25962E-02	0.50100E 00	0.53300E 00	0.46600E 00	
0.10558E-01	-0.10984E-02	0.47500E 00	0.55300E 00	0.47100E 00	
0.10601E-01	-0.18917E-02	0.47600E 00	0.55600E 00	0.47800E 00	
0.24944E-02	0.55190E-05	0.10100E 00	0.54800E 00	0.45100E 00	
0.31956E-01	0.18435E-02	0.23350E 01	0.55000E 00	0.61000E 00	
0.29096E-01	-0.49659E-03	0.25400E 01	0.45200E 00	0.51000E 00	
0.31451E-01	-0.17516E-02	0.24050E 01	0.52400E 00	0.57200E 00	
0.26118E-02	0.17881E-02	0.48900E 00	0.98000E-01	0.51300E 00	
0.69238E-02	0.41361E-02	0.48000E 00	0.48000E 00	0.25500E 01	
0.62809E-02	-0.95091E-03	0.55500E 00	0.29900E 00	0.16450E 01	
0.16712E-01	0.21374E-02	0.59900E 00	0.99600E 00	0.90700E 00	
0.16394E-01	-0.22545E-02	0.43800E 00	0.15230E 01	0.13600E 00	
0.17594E-01	-0.16948E-02	0.47800E 00	0.14800E 01	0.14400E 00	

CORRELATION MATRIX

1.000				
0.777	1.000			
0.772	0.869	1.000		
0.950	0.919	0.840	1.000	

6 STEPS

DEPENDENT	INDEPENDENT		
	1	2	3
0.20100E-01	0.50000E 00	0.27350E 01	0.27000E 00
0.11400E-01	0.48200E 00	0.56000E 00	0.62000E-01
0.13400E-01	0.50100E 00	0.53300E 00	0.46600E 00
0.94600E-02	0.47500E 00	0.55300E 00	0.47100E 00
0.87100E-02	0.47600E 00	0.55600E 00	0.47800E 00
0.25000E-02	0.10100E 00	0.54800E 00	0.45100E 00
0.33800E-01	0.23350E 01	0.55000E 00	0.61000E 00
0.28600E-01	0.25400E 01	0.45200E 00	0.51000E 00
0.29700E-01	0.24050E 01	0.52400E 00	0.57200E 00
0.44000E-02	0.48900E 00	0.98000E-01	0.51300E 00
0.11060E-01	0.48000E 00	0.48000E 00	0.25500E 01
0.53300E-02	0.55500E 00	0.29900E 00	0.16450E 01
0.18850E-01	0.59900E 00	0.99600E 00	0.90700E 00
0.14140E-01	0.43800E 00	0.15230E 01	0.13600E 00
0.15900E-01	0.47800E 00	0.14800E 01	0.14400E 00

MATRIX 1 IS A + SL*0
 MATRIX 2 IS A + SL*1
 MATRIX 3 IS A + SL*0-1

PHI= 0.11983E-02 PARAMETERS	SQRT(PHI)/ND= 0.23078E-02 0.23000E 00	0.55000E 00	LAMBDA= 0.10000E-01 0.40000E-01	0.10300E 01	MATRIX
PHI= 0.49324E-04 PARAMETERS	SQRT(PHI)/ND= 0.46820E-03 0.19307E 00	0.43260E 00	LAMBDA= 0.99999E-02 0.84087E-01	0.87734E 00	MATRIX
PHI= 0.46962E-04 PARAMETERS	SQRT(PHI)/ND= 0.45686E-03 0.19657E 00	0.43360E 00	LAMBDA= 0.99999E-01 0.84582E-01	0.87827E 00	MATRIX
PHI= 0.46447E-04 PARAMETERS	SQRT(PHI)/ND= 0.45435E-03 0.19819E 00	0.43407E 00	LAMBDA= 0.99999E-01 0.84814E-01	0.87870E 00	MATRIX
PHI= 0.46331E-04 PARAMETERS	SQRT(PHI)/ND= 0.45378E-03 0.19895E 00	0.43429E 00	LAMBDA= 0.99999E-01 0.84924E-01	0.87891E 00	MATRIX
PHI= 0.46304E-04 PARAMETERS	SQRT(PHI)/ND= 0.45364E-03 0.19932E 00	0.43440E 00	LAMBDA= 0.99999E-01 0.84977E-01	0.87900E 00	MATRIX
PHI= 0.46297E-04 PARAMETERS	SQRT(PHI)/ND= 0.45361E-03 0.19949E 00	0.43445E 00	LAMBDA= 0.99999E-01 0.85002E-01	0.87905E 00	MATRIX
PHI= 0.46295E-04 PARAMETERS	SQRT(PHI)/ND= 0.45360E-03 0.19957E 00	0.43447E 00	LAMBDA= 0.99999E-01 0.85013E-01	0.87907E 00	MATRIX
PHI= 0.46295E-04 PARAMETERS	SQRT(PHI)/ND= 0.45360E-03 0.19961E 00	0.43448E 00	LAMBDA= 0.99999E-01 0.85019E-01	0.87908E 00	MATRIX
PHI= 0.46295E-04 PARAMETERS	SQRT(PHI)/ND= 0.45360E-03 0.19963E 00	0.43449E 00	LAMBDA= 0.99999E-01 0.85022E-01	0.87908E 00	MATRIX
PHI= 0.46295E-04 PARAMETERS	SQRT(PHI)/ND= 0.45360E-03 0.19964E 00	0.43449E 00	LAMBDA= 0.99999E-01 0.85023E-01	0.87909E 00	MATRIX

ALGORITHM TERMINATED

PHI= 0.46295E-04 PARAMETERS	SQRT(PHI)/ND= 0.45360E-03 0.19964E 00	0.43449E 00	LAMBDA= 0.10000E 04 0.85023E-01	0.87909E 00	MATRIX
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SINGULAR MATRIX

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3	4
		1			
0.19523E-01	0.57620E-03	0.50000E 00	0.27350E 01	0.27000E 00	
0.11381E-01	0.18712E-04	0.48200E 00	0.56000E 00	0.62000E-01	
0.10829E-01	0.25700E-02	0.50100E 00	0.53300E 00	0.46600E 00	
0.10592E-01	-0.11325E-02	0.47500E 00	0.55300E 00	0.47100E 00	
0.10639E-01	-0.19299E-02	0.47600E 00	0.55600E 00	0.47800E 00	
0.25105E-02	-0.10529E-04	0.10100E 00	0.54800E 00	0.45100E 00	
0.31723E-01	0.20763E-02	0.23350E 01	0.55000E 00	0.61000E 00	
0.28690E-01	-0.90647E-04	0.25400E 01	0.45200E 00	0.51000E 00	
0.31149E-01	-0.14496E-02	0.24050E 01	0.52400E 00	0.57200E 00	
0.26076E-02	0.17923E-02	0.48900E 00	0.98000E-01	0.51300E 00	
0.75926E-02	0.34673E-02	0.48000E 00	0.48000E 00	0.25500E 01	

0.66393E-02	-0.13093E-02	0.55500E 00	0.29900E 00	0.16450E 01
0.17134E-01	0.17151E-02	0.59900E 00	0.99600E 00	0.90700E 00
0.16408E-01	-0.22683E-02	0.43800E 00	0.15230E 01	0.13600E 00
0.17600E-01	-0.17009E-02	0.47800E 00	0.14800E 01	0.14400E 00

CORRELATION MATRIX

1.000			
0.772	1.000		
0.756	0.849	1.000	
0.946	0.922	0.820	1.000

11 STEPS

DEPENDENT	INDEPENDENT		
	1	2	3
0.20100E-01	0.50000E 00	0.27350E 01	0.27000E 00
0.11400E-01	0.48200E 00	0.56000E 00	0.62000E-01
0.13400E-01	0.50100E 00	0.53300E 00	0.46600E 00
0.94600E-02	0.47500E 00	0.55300E 00	0.47100E 00
0.87100E-02	0.47600E 00	0.55600E 00	0.47800E 00
0.25000E-02	0.10100E 00	0.54800E 00	0.45100E 00
0.33800E-01	0.23350E 01	0.55000E 00	0.61000E 00
0.28600E-01	0.25400E 01	0.45200E 00	0.51000E 00
0.29700E-01	0.24050E 01	0.52400E 00	0.57200E 00
0.44000E-02	0.48900E 00	0.98000E-01	0.51300E 00
0.11060E-01	0.48000E 00	0.48000E 00	0.25500E 01
0.53300E-02	0.55500E 00	0.29900E 00	0.16450E 01
0.18850E-01	0.59900E 00	0.99600E 00	0.90700E 00
0.14140E-01	0.43800E 00	0.15230E 01	0.13600E 00
0.15900E-01	0.47800E 00	0.14800E 01	0.14400E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.27553E-03 PARAMETERS	SQRT(PHI)/ND= 0.11066E-02 0.17000E 00	0.41000E 00	LAMBDA= 0.10000E-01 0.20000E-01	0.75000E 00	MATRIX
PHI= 0.65924E-04 PARAMETERS	SQRT(PHI)/ND= 0.54129E-03 0.19485E 00	0.41185E 00	LAMBDA= 0.99999E-02 0.81014E-01	0.86287E 00	MATRIX
PHI= 0.63463E-04 PARAMETERS	SQRT(PHI)/ND= 0.53109E-03 0.19609E 00	0.41517E 00	LAMBDA= 0.99999E 01 0.90151E-01	0.86702E 00	MATRIX
PHI= 0.62163E-04 PARAMETERS	SQRT(PHI)/ND= 0.52562E-03 0.19715E 00	0.41816E 00	LAMBDA= 0.99999E 01 0.98953E-01	0.87061E 00	MATRIX
PHI= 0.61692E-04 PARAMETERS	SQRT(PHI)/ND= 0.52362E-03 0.19806E 00	0.42089E 00	LAMBDA= 0.99999E 01 0.10750E 00	0.87376E 00	MATRIX
PHI= 0.61632E-04 PARAMETERS	SQRT(PHI)/ND= 0.52337E-03 0.19817E 00	0.42122E 00	LAMBDA= 0.99999E 02 0.10851E 00	0.87415E 00	MATRIX
PHI= 0.61583E-04 PARAMETERS	SQRT(PHI)/ND= 0.52316E-03 0.19829E 00	0.42154E 00	LAMBDA= 0.99999E 02 0.10951E 00	0.87453E 00	MATRIX
PHI= 0.61543E-04 PARAMETERS	SQRT(PHI)/ND= 0.52299E-03 0.19840E 00	0.42187E 00	LAMBDA= 0.99999E 02 0.11051E 00	0.87491E 00	MATRIX
PHI= 0.61511E-04 PARAMETERS	SQRT(PHI)/ND= 0.52286E-03 0.19850E 00	0.42219E 00	LAMBDA= 0.99999E 02 0.11150E 00	0.87528E 00	MATRIX
PHI= 0.61488E-04 PARAMETERS	SQRT(PHI)/ND= 0.52276E-03 0.19861E 00	0.42250E 00	LAMBDA= 0.99999E 02 0.11249E 00	0.87564E 00	MATRIX
PHI= 0.61473E-04 PARAMETERS	SQRT(PHI)/ND= 0.52270E-03 0.19871E 00	0.42282E 00	LAMBDA= 0.99999E 02 0.11348E 00	0.87600E 00	MATRIX
PHI= 0.61466E-04 PARAMETERS	SQRT(PHI)/ND= 0.52267E-03 0.19882E 00	0.42313E 00	LAMBDA= 0.99999E 02 0.11446E 00	0.87635E 00	MATRIX
PHI= 0.61398E-04 PARAMETERS	SQRT(PHI)/ND= 0.52238E-03 0.19887E 00	0.42316E 00	LAMBDA= 0.99999E 01 0.11448E 00	0.87637E 00	MATRIX
PHI= 0.60774E-04 PARAMETERS	SQRT(PHI)/ND= 0.51972E-03 0.19933E 00	0.42346E 00	LAMBDA= 0.99999E 00 0.11470E 00	0.87656E 00	MATRIX
PHI= 0.57814E-04 PARAMETERS	SQRT(PHI)/ND= 0.50690E-03 0.20203E 00	0.42571E 00	LAMBDA= 0.99999E-01 0.11651E 00	0.87780E 00	MATRIX
PHI= 0.56630E-04 PARAMETERS	SQRT(PHI)/ND= 0.50168E-03 0.20365E 00	0.42753E 00	LAMBDA= 0.99999E-01 0.11815E 00	0.87867E 00	MATRIX
PHI= 0.56184E-04 PARAMETERS	SQRT(PHI)/ND= 0.49971E-03 0.20459E 00	0.42907E 00	LAMBDA= 0.99999E-01 0.11967E 00	0.87931E 00	MATRIX
PHI= 0.56053E-04 PARAMETERS	SQRT(PHI)/ND= 0.49912E-03 0.20510E 00	0.43041E 00	LAMBDA= 0.99999E-01 0.12112E 00	0.87979E 00	MATRIX
PHI= 0.55983E-04 PARAMETERS	SQRT(PHI)/ND= 0.49881E-03 0.20537E 00	0.43056E 00	LAMBDA= 0.99999E-02 0.12115E 00	0.87982E 00	MATRIX

PHI= 0.55707E-04 PARAMETERS	SQRT(PHI)/ND= 0.49758E-03 0.20584E 00	0.43177E 00	LAMBDA= 0.99999E-03 0.12148E 00	0.88002E 00	MATRI
PHI= 0.54933E-04 PARAMETERS	SQRT(PHI)/ND= 0.49411E-03 0.20276E 00	0.43946E 00	LAMBDA= 0.99999E-04 0.12433E 00	0.88090E 00	MATRI
PHI= 0.54780E-04 PARAMETERS	SQRT(PHI)/ND= 0.49342E-03 0.20120E 00	0.44497E 00	LAMBDA= 0.99999E-04 0.12704E 00	0.88142E 00	MATRI
PHI= 0.54737E-04 PARAMETERS	SQRT(PHI)/ND= 0.49323E-03 0.20162E 00	0.44558E 00	LAMBDA= 0.99999E-03 0.12732E 00	0.88150E 00	MATRI
PHI= 0.54732E-04 PARAMETERS	SQRT(PHI)/ND= 0.49320E-03 0.20162E 00	0.44614E 00	LAMBDA= 0.99999E-03 0.12760E 00	0.88156E 00	MATRI
PHI= 0.54731E-04 PARAMETERS	SQRT(PHI)/ND= 0.49320E-03 0.20163E 00	0.44620E 00	LAMBDA= 0.99999E-02 0.12763E 00	0.88157E 00	MATRI
PHI= 0.54731E-04 PARAMETERS	SQRT(PHI)/ND= 0.49320E-03 0.20164E 00	0.44626E 00	LAMBDA= 0.99999E-02 0.12765E 00	0.88157E 00	MATRI
PHI= 0.54731E-04 PARAMETERS	SQRT(PHI)/ND= 0.49320E-03 0.20164E 00	0.44632E 00	LAMBDA= 0.99999E-02 0.12768E 00	0.88158E 00	MATRI
PHI= 0.54731E-04 PARAMETERS	SQRT(PHI)/ND= 0.49320E-03 0.20166E 00	0.44632E 00	LAMBDA= 0.99999E-01 0.12768E 00	0.88158E 00	MATRI
PHI= 0.54731E-04 PARAMETERS	SQRT(PHI)/ND= 0.49320E-03 0.20166E 00	0.44632E 00	LAMBDA= 0.99999E 00 0.12768E 00	0.88158E 00	MATRI
PHI= 0.54731E-04 PARAMETERS	SQRT(PHI)/ND= 0.49320E-03 0.20166E 00	0.44632E 00	LAMBDA= 0.99999E 00 0.12768E 00	0.88158E 00	MATRI

ALGORITHM CONVERGED

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3
		1		
0.19548E-01	0.55148E-03	0.50000E 00	0.27350E 01	0.27000E 00
0.11664E-01	-0.26426E-03	0.48200E 00	0.56000E 00	0.62000E-01
0.10834E-01	0.25650E-02	0.50100E 00	0.53300E 00	0.46600E 00
0.10592E-01	-0.11324E-02	0.47500E 00	0.55300E 00	0.47100E 00
0.10635E-01	-0.19254E-02	0.47600E 00	0.55600E 00	0.47800E 00
0.25108E-02	-0.10859E-04	0.10100E 00	0.54800E 00	0.45100E 00
0.31653E-01	0.21463E-02	0.23350E 01	0.55000E 00	0.61000E 00
0.28781E-01	-0.18197E-03	0.25400E 01	0.45200E 00	0.51000E 00
0.31142E-01	-0.14425E-02	0.24050E 01	0.52400E 00	0.57200E 00
0.26064E-02	0.17935E-02	0.48900E 00	0.98000E-01	0.51300E 00
0.68252E-02	0.42347E-02	0.48000E 00	0.48000E 00	0.25500E 01
0.62162E-02	-0.88621E-03	0.55500E 00	0.29900E 00	0.16450E 01
0.16749E-01	0.21000E-02	0.59900E 00	0.99600E 00	0.90700E 00
0.16604E-01	-0.24642E-02	0.43800E 00	0.15230E 01	0.13600E 00
0.17810E-01	-0.19100E-02	0.47800E 00	0.14800E 01	0.14400E 00

CORRELATION MATRIX

1.000			
0.770	1.000		
0.767	0.870	1.000	
0.947	0.919	0.839	1.000

29 STEPS

DEPENDENT	INDEPENDENT		
	1	2	3
C.20100E-01	0.50000E 00	0.27350E 01	0.27000E 00
C.11400E-01	0.48200E 00	0.56000E 00	0.62000E-01
C.13400E-01	0.50100E 00	0.53300E 00	0.46600E 00
C.94600E-02	0.47500E 00	0.55300E 00	0.47100E 00
C.87100E-02	0.47600E 00	0.55600E 00	0.47800E 00
C.25000E-02	0.10100E 00	0.54800E 00	0.45100E 00
C.33800E-01	0.23350E 01	0.55000E 00	0.61000E 00
C.28600E-01	0.25400E 01	0.45200E 00	0.51000E 00
C.29700E-01	0.24050E 01	0.52400E 00	0.57200E 00
C.44000E-02	0.48900E 00	0.98000E-01	0.51300E 00
C.11060E-01	0.48000E 00	0.48000E 00	0.25500E 01
C.53300E-02	0.55500E 00	0.29900E 00	0.16450E 01
C.18850E-01	0.59900E 00	0.99600E 00	0.90700E 00
C.14140E-01	0.43800E 00	0.15230E 01	0.13600E 00
C.15900E-01	0.47800E 00	0.14800E 01	0.14400E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.41275E-04 PARAMETERS	SQRT(PHI)/ND= 0.42830E-03 0.20000E 00	0.43000E 00	LAMBDA= 0.10000E-01 0.50000E-01	0.88000E 00	MATRI
PHI= 0.40965E-04 PARAMETERS	SQRT(PHI)/ND= 0.42669E-03 0.19956E 00	0.42947E 00	LAMBDA= 0.10000E 02 0.51311E-01	0.87887E 00	MATRI
PHI= 0.40921E-04 PARAMETERS	SQRT(PHI)/ND= 0.42646E-03 0.19922E 00	0.42913E 00	LAMBDA= 0.99999E 01 0.52971E-01	0.87802E 00	MATRI
PHI= 0.40606E-04 PARAMETERS	SQRT(PHI)/ND= 0.42481E-03 0.19797E 00	0.42876E 00	LAMBDA= 0.99999E-01 0.52781E-01	0.87767E 00	MATRI
PHI= 0.40533E-04 PARAMETERS	SQRT(PHI)/ND= 0.42443E-03 0.19737E 00	0.42858E 00	LAMBDA= 0.99999E-01 0.52690E-01	0.87751E 00	MATRI
PHI= 0.40516E-04 PARAMETERS	SQRT(PHI)/ND= 0.42434E-03 0.19709E 00	0.42850E 00	LAMBDA= 0.99999E-01 0.52647E-01	0.87743E 00	MATRI
PHI= 0.40512E-04 PARAMETERS	SQRT(PHI)/ND= 0.42432E-03 0.19695E 00	0.42846E 00	LAMBDA= 0.99999E-01 0.52626E-01	0.87739E 00	MATRI
PHI= 0.40511E-04 PARAMETERS	SQRT(PHI)/ND= 0.42432E-03 0.19689E 00	0.42844E 00	LAMBDA= 0.99999E-01 0.52617E-01	0.87737E 00	MATRI
PHI= 0.40510E-04 PARAMETERS	SQRT(PHI)/ND= 0.42432E-03 0.19686E 00	0.42843E 00	LAMBDA= 0.99999E-01 0.52612E-01	0.87736E 00	MATRI
PHI= 0.40510E-04 PARAMETERS	SQRT(PHI)/ND= 0.42432E-03 0.19685E 00	0.42843E 00	LAMBDA= 0.99999E-01 0.52610E-01	0.87736E 00	MATRI

ALGORITHM TERMINATED

PHI= 0.40510E-04 PARAMETERS	SQRT(PHI)/ND= 0.42432E-03 0.19685E 00	0.42843E 00	LAMBDA= 0.10000E 04 0.52610E-01	0.87736E 00	MATRI
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SINGULAR MATRIX

DEPENDENT	DIFFERENCE	INDEPENDENT		
		1	2	3
C.19390E-01	0.70966E-03	0.50000E 00	0.27350E 01	0.27000E 00
C.11155E-01	0.24473E-03	0.48200E 00	0.56000E 00	0.62000E-01
C.10817E-01	0.25822E-02	0.50100E 00	0.53300E 00	0.46600E 00
C.10582E-01	-0.11229E-02	0.47500E 00	0.55300E 00	0.47100E 00
C.10633E-01	-0.19237E-02	0.47600E 00	0.55600E 00	0.47800E 00
C.25059E-02	-0.59669E-05	0.10100E 00	0.54800E 00	0.45100E 00
C.31847E-01	0.19524E-02	0.23350E 01	0.55000E 00	0.61000E 00
C.28699E-01	-0.99297E-04	0.25400E 01	0.45200E 00	0.51000E 00
C.31228E-01	-0.15284E-02	0.24050E 01	0.52400E 00	0.57200E 00
C.26116E-02	0.17883E-02	0.48900E 00	0.98000E-01	0.51300E 00
C.82871E-02	0.27728E-02	0.48000E 00	0.48000E 00	0.25500E 01
C.70057E-02	-0.16757E-02	0.55500E 00	0.29900E 00	0.16450E 01
C.17410E-01	0.14395E-02	0.59900E 00	0.99600E 00	0.90700E 00
C.16193E-01	-0.20536E-02	0.43800E 00	0.15230E 01	0.13600E 00

DEPENDENT	INDEPENDENT		
	1	2	3
C.20100E-01	0.50000E 00	0.27350E 01	0.27000E 00
0.11400E-01	0.48200E 00	0.56000E 00	0.62000E-01
0.13400E-01	0.50100E 00	0.53300E 00	0.46600E 00
0.94600E-02	0.47500E 00	0.55300E 00	0.47100E 00
0.87100E-02	0.47600E 00	0.55600E 00	0.47800E 00
0.25000E-02	0.10100E 00	0.54800E 00	0.45100E 00
0.33800E-01	0.23350E 01	0.55000E 00	0.61000E 00
0.28600E-01	0.25400E 01	0.45200E 00	0.51000E 00
0.29700E-01	0.24050E 01	0.52400E 00	0.57200E 00
0.44000E-02	0.48900E 00	0.98000E-01	0.51300E 00
0.11060E-01	0.48000E 00	0.48000E 00	0.25500E 01
0.53300E-02	0.55500E 00	0.29900E 00	0.16450E 01
0.18850E-01	0.59900E 00	0.99600E 00	0.90700E 00
C.14140E-01	0.43800E 00	0.15230E 01	0.13600E 00
0.15900E-01	0.47800E 00	0.14800E 01	0.14400E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.41085E-04 PARAMETERS	SQRT(PHI)/ND= 0.42732E-03 0.20000E 00	0.43000E 00	LAMBDA= 0.10000E-01 0.30000E-01	0.88000E 00	MATRIX
PHI= 0.38322E-04 PARAMETERS	SQRT(PHI)/ND= 0.41270E-03 0.19700E 00	0.42576E 00	LAMBDA= 0.10000E 01 0.37648E-01	0.87218E 00	MATRIX
PHI= 0.38321E-04 PARAMETERS	SQRT(PHI)/ND= 0.41269E-03 0.19692E 00	0.42574E 00	LAMBDA= 0.99999E-01 0.37634E-01	0.87215E 00	MATRIX
PHI= 0.38320E-04 PARAMETERS	SQRT(PHI)/ND= 0.41269E-03 0.19687E 00	0.42573E 00	LAMBDA= 0.99999E-01 0.37628E-01	0.87214E 00	MATRIX
PHI= 0.38320E-04 PARAMETERS	SQRT(PHI)/ND= 0.41269E-03 0.19686E 00	0.42572E 00	LAMBDA= 0.99999E-01 0.37625E-01	0.87213E 00	MATRIX
PHI= 0.38320E-04 PARAMETERS	SQRT(PHI)/ND= 0.41269E-03 0.19685E 00	0.42572E 00	LAMBDA= 0.99999E-01 0.37623E-01	0.87213E 00	MATRIX
PHI= 0.38320E-04 PARAMETERS	SQRT(PHI)/ND= 0.41269E-03 0.19684E 00	0.42572E 00	LAMBDA= 0.99999E-01 0.37622E-01	0.87213E 00	MATRIX

ALGORITHM TERMINATED

PHI= 0.38320E-04 PARAMETERS	SQRT(PHI)/ND= 0.41269E-03 0.19684E 00	0.42572E 00	LAMBDA= 0.10000E 04 0.37622E-01	0.87213E 00	MATRIX
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SINGULAR MATRIX

DEPENDENT	DIFFERENCE	INDEPENDENT			
		1	2	3	4
C.19346E-01	0.75390E-03	0.50000E 00	0.27350E 01	0.27000E 00	
0.11058E-01	0.34115E-03	0.48200E 00	0.56000E 00	0.62000E-01	
0.10819E-01	0.25803E-02	0.50100E 00	0.53300E 00	0.46600E 00	
C.10586E-01	-0.11264E-02	0.47500E 00	0.55300E 00	0.47100E 00	
0.10638E-01	-0.19288E-02	0.47600E 00	0.55600E 00	0.47800E 00	
C.25074E-02	-0.74608E-05	0.10100E 00	0.54800E 00	0.45100E 00	
C.31847E-01	0.19520E-02	0.23350E 01	0.55000E 00	0.61000E 00	
C.28641E-01	-0.41995E-04	0.25400E 01	0.45200E 00	0.51000E 00	
0.31205E-01	-0.15054E-02	0.24050E 01	0.52400E 00	0.57200E 00	
0.26151E-02	C.17848E-02	0.48900E 00	0.98000E-01	0.51300E 00	
C.86559E-02	0.24040E-02	0.48000E 00	0.48000E 00	0.25500E 01	
0.71939E-02	-0.18639E-02	0.55500E 00	0.29900E 00	0.16450E 01	
0.17554E-01	0.12957E-02	0.59900E 00	0.99600E 00	0.90700E 00	
C.16108E-01	-0.19686E-02	0.43800E 00	0.15230E 01	0.13600E 00	
C.17284E-01	-0.13841E-02	0.47800E 00	0.14800E 01	0.14400E 00	

CORRELATION MATRIX

1.000				
0.775	1.000			
0.740	0.819	1.000		
0.944	0.924	0.793	1.000	

DEPENDENT	INDEPENDENT		2	3
	1			
0.20100E-01	0.50000E 00	0.27350E 01	0.27000E 00	
0.11400E-01	0.48200E 00	0.56000E 00	0.62000E -01	
0.13400E-01	0.50100E 00	0.53300E 00	0.46600E 00	
0.94600E-02	0.47500E 00	0.55300E 00	0.47100E 00	
0.87100E-02	0.47600E 00	0.55600E 00	0.47800E 00	
0.25000E-02	0.10100E 00	0.54800E 00	0.45100E 00	
0.33800E-01	0.23350E 01	0.55000E 00	0.61000E 00	
0.28600E-01	0.25400E 01	0.45200E 00	0.51000E 00	
0.29700E-01	0.24050E 01	0.52400E 00	0.57200E 00	
0.44000E-02	0.48900E 00	0.98000E -01	0.51300E 00	
0.11060E-01	0.48000E 00	0.48000E 00	0.25500E 01	
0.53300E-02	0.55500E 00	0.29900E 00	0.16450E 01	
0.18850E-01	0.59900E 00	0.99600E 00	0.90700E 00	
0.14140E-01	0.43800E 00	0.15230E 01	0.13600E 00	
0.15900E-01	0.47800E 00	0.14800E 01	0.14400E 00	

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.51951E-04 PARAMETERS	SQRT(PHI)/ND= 0.48051E-03 0.19700E 00 0.42600E 00	LAMBDA= 0.10000E-01 0.38000E-01 0.92000E 00	MATRIX
PHI= 0.39745E-04 PARAMETERS	SQRT(PHI)/ND= 0.42029E-03 0.19244E 00 0.41852E 00	LAMBDA= 0.10000E 01 0.43698E-01 0.90611E 00	MATRIX
PHI= 0.37913E-04 PARAMETERS	SQRT(PHI)/ND= 0.41049E-03 0.19244E 00 0.41852E 00	LAMBDA= 0.99999E-02 0.30649E-01 0.88208E 00	MATRIX
PHI= 0.37501E-04 PARAMETERS	SQRT(PHI)/ND= 0.40825E-03 0.19244E 00 0.41853E 00	LAMBDA= 0.99999E 00 0.30649E-01 0.88822E 00	MATRIX
PHI= 0.37466E-04 PARAMETERS	SQRT(PHI)/ND= 0.40806E-03 0.19245E 00 0.41854E 00	LAMBDA= 0.99999E 00 0.30649E-01 0.89001E 00	MATRIX
PHI= 0.37437E-04 PARAMETERS	SQRT(PHI)/ND= 0.40790E-03 0.19245E 00 0.41854E 00	LAMBDA= 0.99999E 00 0.30445E-01 0.89000E 00	MATRIX
PHI= 0.37328E-04 PARAMETERS	SQRT(PHI)/ND= 0.40731E-03 0.19245E 00 0.41854E 00	LAMBDA= 0.99999E 00 0.29648E-01 0.88999E 00	MATRIX
PHI= 0.37328E-04 PARAMETERS	SQRT(PHI)/ND= 0.40731E-03 0.19243E 00 0.41854E 00	LAMBDA= 0.99999E-02 0.29648E-01 0.88996E 00	MATRIX
PHI= 0.37327E-04 PARAMETERS	SQRT(PHI)/ND= 0.40731E-03 0.19241E 00 0.41854E 00	LAMBDA= 0.99999E-02 0.29648E-01 0.88991E 00	MATRIX
PHI= 0.37059E-04 PARAMETERS	SQRT(PHI)/ND= 0.40584E-03 0.19242E 00 0.41854E 00	LAMBDA= 0.99999E 00 0.27589E-01 0.88990E 00	MATRIX
PHI= 0.36665E-04 PARAMETERS	SQRT(PHI)/ND= 0.40368E-03 0.19242E 00 0.41854E 00	LAMBDA= 0.99999E-02 0.24106E-01 0.88990E 00	MATRIX
PHI= 0.36246E-04 PARAMETERS	SQRT(PHI)/ND= 0.40136E-03 0.19242E 00 0.41854E 00	LAMBDA= 0.99999E-02 -0.10548E-02 0.88990E 00	MATRIX
PHI= 0.34454E-04 PARAMETERS	SQRT(PHI)/ND= 0.39132E-03 0.19069E 00 0.41523E 00	LAMBDA= 0.99999E 00 0.11631E-02 0.88488E 00	MATRIX
PHI= 0.34096E-04 PARAMETERS	SQRT(PHI)/ND= 0.38928E-03 0.19069E 00 0.41523E 00	LAMBDA= 0.99999E-02 -0.45853E-02 0.87707E 00	MATRIX
PHI= 0.34076E-04 PARAMETERS	SQRT(PHI)/ND= 0.38916E-03 0.19069E 00 0.41523E 00	LAMBDA= 0.99999E 00 -0.45852E-02 0.87843E 00	MATRIX
PHI= 0.34074E-04 PARAMETERS	SQRT(PHI)/ND= 0.38915E-03 0.19069E 00 0.41523E 00	LAMBDA= 0.99999E 00 -0.45852E-02 0.87882E 00	MATRIX
PHI= 0.34074E-04 PARAMETERS	SQRT(PHI)/ND= 0.38915E-03 0.19068E 00 0.41523E 00	LAMBDA= 0.99999E-02 -0.45852E-02 0.87879E 00	MATRIX
PHI= 0.34021E-04 PARAMETERS	SQRT(PHI)/ND= 0.38885E-03 0.19068E 00 0.41523E 00	LAMBDA= 0.99999E 00 -0.56529E-02 0.87879E 00	MATRIX
PHI= 0.33909E-04 PARAMETERS	SQRT(PHI)/ND= 0.38821E-03 0.19068E 00 0.41523E 00	LAMBDA= 0.99999E-02 -0.92092E-02 0.87879E 00	MATRIX

PHI= 0.33895E-04 PARAMETERS	SQRT(PHI)/ND= 0.38813E-03 0.19060E 00 0.41507E 00	LAMBDA= 0.99999E 01 -0.89563E-02 0.87858E 00	MATR
PHI= 0.33893E-04 PARAMETERS	SQRT(PHI)/ND= 0.38812E-03 0.19054E 00 0.41494E 00	LAMBDA= 0.99999E 01 -0.86372E-02 0.87843E 00	MATR
PHI= 0.33754E-04 PARAMETERS	SQRT(PHI)/ND= 0.38732E-03 0.19054E 00 0.41494E 00	LAMBDA= 0.99999E-02 -0.12720E-01 0.87421E 00	MATR
PHI= 0.33751E-04 PARAMETERS	SQRT(PHI)/ND= 0.38730E-03 0.19054E 00 0.41494E 00	LAMBDA= 0.99999E-02 -0.12749E-01 0.87480E 00	MATR
PHI= 0.33711E-04 PARAMETERS	SQRT(PHI)/ND= 0.38707E-03 0.19054E 00 0.41494E 00	LAMBDA= 0.99999E-02 -0.14530E-01 0.87366E 00	MATR
PHI= 0.33678E-04 PARAMETERS	SQRT(PHI)/ND= 0.38688E-03 0.19054E 00 0.41494E 00	LAMBDA= 0.99999E-02 -0.16585E-01 0.87260E 00	MATR
PHI= 0.33678E-04 PARAMETERS	SQRT(PHI)/ND= 0.38688E-03 0.19054E 00 0.41494E 00	LAMBDA= 0.99999E 02 -0.16573E-01 0.87259E 00	MATR
PHI= 0.33678E-04 PARAMETERS	SQRT(PHI)/ND= 0.38688E-03 0.19053E 00 0.41493E 00	LAMBDA= 0.99999E 02 -0.16559E-01 0.87259E 00	MATR
PHI= 0.33678E-04 PARAMETERS	SQRT(PHI)/ND= 0.38688E-03 0.19053E 00 0.41492E 00	LAMBDA= 0.99999E 02 -0.16546E-01 0.87259E 00	MATR
PHI= 0.33658E-04 PARAMETERS	SQRT(PHI)/ND= 0.38677E-03 0.19053E 00 0.41492E 00	LAMBDA= 0.99999E-02 -0.19410E-01 0.87110E 00	MATR
PHI= 0.33649E-04 PARAMETERS	SQRT(PHI)/ND= 0.38672E-03 0.19042E 00 0.41437E 00	LAMBDA= 0.99999E 00 -0.19066E-01 0.87128E 00	MATR
PHI= 0.33649E-04 PARAMETERS	SQRT(PHI)/ND= 0.38672E-03 0.19042E 00 0.41437E 00	LAMBDA= 0.99999E 03 -0.19065E-01 0.87128E 00	MATR
PHI= 0.33646E-04 PARAMETERS	SQRT(PHI)/ND= 0.38670E-03 0.19042E 00 0.41437E 00	LAMBDA= 0.99999E-02 -0.20019E-01 0.87187E 00	MATR
PHI= 0.33631E-04 PARAMETERS	SQRT(PHI)/ND= 0.38661E-03 0.18960E 00 0.41160E 00	LAMBDA= 0.99999E-01 -0.18565E-01 0.87580E 00	MATR
PHI= 0.33630E-04 PARAMETERS	SQRT(PHI)/ND= 0.38660E-03 0.18963E 00 0.41168E 00	LAMBDA= 0.99999E 01 -0.18312E-01 0.87597E 00	MATR
PHI= 0.33629E-04 PARAMETERS	SQRT(PHI)/ND= 0.38660E-03 0.18966E 00 0.41174E 00	LAMBDA= 0.99999E 01 -0.18064E-01 0.87613E 00	MATR
PHI= 0.33610E-04 PARAMETERS	SQRT(PHI)/ND= 0.38649E-03 0.18966E 00 0.41175E 00	LAMBDA= 0.99999E 00 -0.18064E-01 0.87745E 00	MATR
PHI= 0.33610E-04 PARAMETERS	SQRT(PHI)/ND= 0.38649E-03 0.18966E 00 0.41175E 00	LAMBDA= 0.99999E 03 -0.18062E-01 0.87745E 00	MATR
PHI= 0.33608E-04 PARAMETERS	SQRT(PHI)/ND= 0.38648E-03 0.18966E 00 0.41175E 00	LAMBDA= 0.99999E-02 -0.18125E-01 0.87768E 00	MATR
PHI= 0.33598E-04 PARAMETERS	SQRT(PHI)/ND= 0.38642E-03 0.18966E 00 0.41175E 00	LAMBDA= 0.99999E-02 -0.19730E-01 0.87768E 00	MATR
PHI= 0.33591E-04 PARAMETERS	SQRT(PHI)/ND= 0.38638E-03 0.18948E 00 0.41131E 00	LAMBDA= 0.99999E 00 -0.19279E-01 0.87773E 00	MATR

ALGORITHM TERMINATED

PHI= 0.33591E-04 PARAMETERS	SQRT(PHI)/ND= 0.38638E-03 0.18948E 00 0.41131E 00	LAMBDA= 0.99999E 04 -0.19279E-01 0.87773E 00	MATR
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DEPENDENT	DIFFERENCE	INDEPENDENT	2	3
		1		
0.19075E-01	0.10241E-02	0.50000E 00	0.27350E 01	0.27000E 00
0.10589E-01	0.81046E-03	0.48200E 00	0.56000E 00	0.62000E-01
0.10723E-01	0.26767E-02	0.50100E 00	0.53300E 00	0.46600E 00
0.10496E-01	-0.10366E-02	0.47500E 00	0.55300E 00	0.47100E 00
0.10555E-01	-0.18450E-02	0.47600E 00	0.55600E 00	0.47800E 00
0.24789E-02	0.21010E-04	0.10100E 00	0.54800E 00	0.45100E 00
0.32000E-01	0.17995E-02	0.23350E 01	0.55000E 00	0.61000E 00
0.28591E-01	0.85234E-05	0.25400E 01	0.45200E 00	0.51000E 00
0.31276E-01	-0.15769E-02	0.24050E 01	0.52400E 00	0.57200E 00
0.25990E-02	0.18009E-02	0.48900E 00	0.98000E-01	0.51300E 00

0.10263E-01	0.79673E-03	0.48000E 00	0.48000E 00	0.25500E 01	86.
0.79302E-02	-0.26002E-02	0.55500E 00	0.29900E 00	0.16450E 01	
0.18001E-01	0.84806E-03	0.59900E 00	0.99600E 00	0.90700E 00	
0.15664E-01	-0.15241E-02	0.43800E 00	0.15230E 01	0.13600E 00	
0.16813E-01	-0.91359E-03	0.47800E 00	0.14800E 01	0.14400E 00	

CORRELATION MATRIX

1.000			
0.785	1.000		
0.718	0.774	1.000	
0.945	0.929	0.753	1.000

40 STEPS

PAGE 1 11/02/72
 // JOB F 1001 2002 3003 4004 F 2
 LOG DRIVE CART SPEC CART AVAIL PHY DRIVE
 0000 000F 000F 0000
 0001 1001 1001 0001
 0002 2002 2002 0002
 0003 3003 3003 0003
 0004 4004 4004 0004
 V2 M09 ACTUAL 8K CONFIG 8K
 USER - WRM PROGRAM NAME - SYNT GROUP - CSRD

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// FOR
*ONE WORD INTEGERS
*LIST ALL
*IOCS(CARD,1403 PRINTER)
C HYDROGENATION OF CODIMER
C PROGRAM TO CALC ERROR AFTER FINDING CONSTANTS
C MECHANISM - NO DISSOCIATION OF HYDROGEN
C
C REAL KH,KU,KS
C DIMENSION PH(20),PU(20),PS(20),REXP(20),RCALC(20),DIFF(20)
C
C ICRD=2
C LPRT=5
C ERROR = 0.0
C PHI=0.0
C
C **** READ CONSTANTS ****
C
C READ(ICRD,100) KH,KU,KS,EK
C
C L=0
C 2 L=L+1
C READ(ICRD,102) REXP(L),PH(L),PU(L),PS(L)
C IF( PH(L) ) 60,30,20
C 20 DENOM = 1.+ KH*PH(L) + KU*PU(L) + KS*PS(L)
C RCALC(L) = EK*KH*KU*PH(L)*PU(L) / DENOM**2
C DIFF(L) = ( REXP(L) - RCALC(L) ) / RCALC(L) * 100.
C PHI = PHI + ( RCALC(L) - REXP(L) )**2
C GO TO 2
C 30 KOUNT = L-1
C WRITE(LPRT,110)
C WRITE(LPRT,111) KH
C WRITE(LPRT,112) KU
C WRITE(LPRT,113) KS
C WRITE(LPRT,114) EK
C WRITE(LPRT,120)
C DO 50 L = 1,KOUNT
C ERROR = ERROR + ABS(DIFF(L))
C 50 WRITE(LPRT,130) L,RCALC(L),REXP(L),PH(L),PU(L),PS(L),DIFF(L)
C XNUM=KOUNT
C ERROR = ERROR/XNUM
C WRITE(LPRT,140) PHI, ERROR
C 60 CALL EXIT
C
C 100 FORMAT( 4F15.0 )
C 102 FORMAT( 10X,4F10.0 )
C 110 FORMAT( 1H1 )
C 111 FORMAT( 6H KH = , F6.4 )
C 112 FORMAT( 6H KU = , F6.4 )
C 113 FORMAT( 6H KS = , F6.4 )
C 114 FORMAT( 6H EK = , F6.4 / )
C 120 FORMAT( 3X,50H CALC EXPER PH PU PS /
C 1 3X,20H RXN RATE RXN RATE ,35X,10H PCT ERROR )
C 130 FORMAT( 1X,12,5F10.5,F10.1 )
C 140 FORMAT( // 18H PHI = , F10.6
C 1 / 18H AVG PCT ERROR = , F10.1 )
C
C END
VARIABLE ALLOCATIONS
PH(R )=0026-0000 PU(R )=004E-0028 PS(R )=0076-0050 REXP(R )=
KH(R )=00F0 KU(R )=00F2 KS(R )=00F4 ERROR(R )=
DENOM(R )=00FC XNUM(R )=00FE ICRD(I )=0104 LPRT(I )=
STATEMENT ALLOCATIONS
100 =0114 102 =0117 110 =0118 111 =011E 112 =0124 113 =012A
2 =01BD 20 =01DC 30 =0229 50 =0264 60 =0294

```

KH = 0.3440
 KU = 0.5160
 KS = 0.5140
 EK = 0.6990

No dissociation of H₂

200°C

	CALC	EXPER	PH	PU	PS	PCT ERROR
	RXN RATE	RXN RATE				
1	0.00273	0.00353	0.48200	0.10000	0.50800	29.0 .00080
2	0.02832	0.02500	2.45900	0.52700	0.51500	-11.7 -.00332
3	0.02841	0.03200	2.45000	0.53000	0.51500	12.5 .00359
4	0.00394	0.00553	0.47700	0.49400	2.53800	40.2 .00154
5	0.01206	0.00870	0.51400	0.54000	0.45500	-27.9 -.00326
6	0.01133	0.01392	0.47300	0.55200	0.47300	22.8 .00259
7	0.01135	0.00960	0.47000	0.55800	0.47300	-15.4 -.00175
8	0.00301	0.00514	0.10400	0.56200	0.44000	70.7 .00213
9	0.02114	0.01920	0.45000	2.84000	0.23000	-9.1 -.00194
10	0.01900	0.02060	0.40900	2.81000	0.28900	8.3 .00160
11	0.01327	0.01310	0.48400	1.07500	0.94200	-1.3 -.00017
12	0.01722	0.01860	0.35700	1.59000	0.15300	7.9 .00138

PHI = 0.000060
 AVG PCT ERROR = 21.4

Check calculation

$$r_2 = \frac{EK K_H K_U P_H P_U}{(1 + K_H P_H + K_U P_U + K_S P_S)^2}$$

$$\frac{(0.699)(0.344)(0.516)(2.459)(.527)}{(1 + (.344)(2.459) + (.516)(.527) + (.514)(.515))^2}$$

$$\frac{0.16078}{(1 + 0.8459 + 0.2719 + 0.2647)^2} = \frac{0.16078}{(2.3825)^2} = 0.02832 \checkmark OK$$

Experimental Data - Parameters from Non-linear Regression

89.1

275°C

No dissociation of H₂

KH = 0.2380
 KU = 0.5890
 KS = 0.2320
 EK = 0.9420

	CALC	EXPER	PH	PU	PS	x 10 ⁻⁵	
	RXN RATE	RXN RATE				PCT	ERROR
1	0.00383	0.00298	0.47800	0.10200	0.52500	-22.3	-85
2	0.04213	0.03890	2.50500	0.51800	0.49700	-7.6	-323
3	0.04216	0.04500	2.50000	0.51700	0.48500	6.7	284
4	0.01976	0.02060	0.42500	2.77000	0.31000	4.2	84
5	0.02020	0.01850	0.43300	2.80000	0.27000	-8.4	-170
6	0.01704	0.01800	0.48900	0.56200	0.05100	5.6	96
7	0.01555	0.01030	0.54600	0.50600	0.44600	-33.7	-525
8	0.01434	0.01215	0.46900	0.55600	0.47500	-15.3	-219
9	0.00339	0.00705	0.10000	0.54000	0.46400	107.7	366
10	0.00657	0.00824	0.42200	0.46200	2.61500	25.3	167
11	0.00755	0.00734	0.46700	0.48500	2.55500	-2.8	-21
12	0.03214	0.03190	1.49500	0.51100	0.49500	-0.7	-24
13	0.03988	0.04350	1.22200	0.77600	0.10300	9.0	370

PHI = 0.000085
 AVG PCT ERROR = 19.2

Experimental Data - Parameters from Non-linear Regression

no dissociation of H₂

90.

KH = 0.1910
KU = 0.4150
KS = 0.0010
EK = 0.8890

325°C

	CALC	EXPER	PH	PU	PS	PCT ERROR	
	RXN RATE	RXN RATE					x10 ⁵
1	0.01936	0.02010	0.50000	2.73500	0.27000	3.8	71
2	0.01084	0.01140	0.48200	0.56000	0.06200	5.1	50
3	0.01084	0.01340	0.50100	0.53300	0.46600	23.5	25
4	0.01061	0.00946	0.47500	0.55300	0.47100	-10.8	-11
5	0.01066	0.00871	0.47600	0.55600	0.47800	-18.3	-19
6	0.00250	0.00250	0.10100	0.54800	0.45100	-0.2	0
7	0.03226	0.03380	2.33500	0.55000	0.61000	4.7	15
8	0.02889	0.02860	2.54000	0.45200	0.51000	-1.0	-2
9	0.03156	0.02970	2.40500	0.52400	0.57200	-5.8	-18
10	0.00262	0.00440	0.48900	0.09800	0.51300	67.7	17
11	0.00970	0.01106	0.48000	0.48000	2.55500	13.9	12
12	0.00770	0.00533	0.55500	0.29900	1.64500	-30.8	-23
13	0.01799	0.01885	0.59900	0.99600	0.90700	4.7	8
14	0.01596	0.01414	0.43800	1.52300	0.13600	-11.4	-18
15	0.01713	0.01590	0.47800	1.48000	0.14400	-7.2	-12

PHI = 0.000034
AVG PCT ERROR = 13.9

MECHANISM (d)

SYNTHETIC DATA

```
// JOB          F 1001 2002 3003 4004      F 2002
LOG DRIVE      CART SPEC      CART AVAIL  PHY DRIVE
0000           000F           000F        0000
0001           1001           1001        0001
0002           2002           2002        0002
0003           3003           3003        0003
0004           4004           4004        0004
```

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - SYN GROUP - CSR

```
// FOR
*ONE WORD INTEGERS
*LIST ALL
*LOCS(CARD,1403 PRINTER)
C HYDROGENATION OF CODIMER
C PROGRAM TO GENERATE REACTION RATES USING ARBITRARY CONSTANTS
C MODEL - NO DISSOCIATION OF HYDROGEN
C
REAL KH, KV, KS
DIMENSION PH(20),PV(20),PS(20),RR(20)
C
ICRD = 2
LPRT = 5
C
***** READ ARBITRARY VALUES FOR PARAMETERS
C
READ(ICRD,102) KH,KV,KS,A
WRITE(LPRT,104) KH,KV,KS,A
C
L=0
2 L=L+1
READ(ICRD,100) PH(L),PV(L),PS(L)
IF( PH(L) ) 10,30,20
20 DENOM = (1 + KH*PH(L) + KV*PV(L) + KS*PS(L) )
RR(L) = A*KH*KV*PH(L)*PV(L) / DENOM**2
GO TO 2
30 KOUNT =L-1
DO 50 L=1,KOUNT
WRITE(ICRD,106)L,RR(L),PH(L),PV(L),PS(L)
50 WRITE(LPRT,102) RR(L),PH(L),PV(L),PS(L)
10 CALL EXLT
C
100 FORMAT( 15X,3F15.4 )
102 FORMAT( 4F15.6 )
104 FORMAT(5H1 KH ,F10.4/5H KU ,F10.4/5H KS ,F10.4/5H EK ,F10.4
1 /// )
106 FORMAT( 12,8X,4F10.6 )
END
VARIABLE ALLOCATIONS
PH(R )=0026-0000 PV(R )=004E-0028 PS(R )=0076-0050 RR(R )=
KS(R )=00A4 A(R )=00A6 DENOM(R )=00A8 ICRD(I )=
KOUNT(I )=00B3
STATEMENT ALLOCATIONS
100 =00BA 102 =00BE 104 =00C1 106 =00DC 2 =011B 20 =0138
FEATURES SUPPORTED
ONE WORD INTEGERS
LOCS
CALLED SUBPROGRAMS
FADD FMPY FMPYX FLD FLDX FSTO FSTOX FDVR FAXI
SIOFX SIOF SIOI SUBSC PRNZ
INTEGER CONSTANTS
2=00B6 5=00B7 0=00B8 1=00B9
CORE REQUIREMENTS FOR
COMMON 0 VARIABLES 182 PROGRAM 242
END OF COMPILATION
// XEQ
```

No DISSOCIATION OF H₂

Synthetic Reaction Rates with no limit

92.

200°C

KH 0.4100
KU 0.5520
KS 0.3670
EK 0.5770

γ	P_H	P_O	P_S
0.003038	0.482000	0.100000	0.508000
0.027335	2.459000	0.527000	0.515000
0.027435	2.450000	0.530000	0.515000
0.005343	0.477000	0.494000	2.538000
0.012906	0.514000	0.540000	0.455000
0.012192	0.473000	0.552000	0.473000
0.012216	0.470000	0.558000	0.473000
0.003328	0.104000	0.562000	0.440000
0.020741	0.450000	2.840000	0.230000
0.018807	0.409000	2.810000	0.289000
0.014870	0.484000	1.075000	0.942000
0.017129	0.357000	1.590000	0.153000

KH 0.2500
KU 0.5810
KS 0.1900
EK 0.8830

275²

93.

0.003825	0.478000	0.102000	0.525000
0.040719	2.505000	0.518000	0.497000
0.040725	2.500000	0.517000	0.485000
0.019614	0.425000	2.770000	0.310000
0.020028	0.433000	2.800000	0.270000
0.016570	0.489000	0.562000	0.051000
0.015433	0.546000	0.506000	0.446000
0.014277	0.469000	0.556000	0.475000
0.003401	0.100000	0.540000	0.464000
0.007144	0.422000	0.462000	2.615000
0.008184	0.467000	0.485000	2.555000
0.031463	1.495000	0.511000	0.495000
0.038562	1.222000	0.776000	0.103000

NO DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE RR
 RESIDUAL STANDARD DEVIATION 0.0024
 STANDARD ERROR OF THE MEAN 0.0007
 MULTIPLE R 0.9999
 MULTIPLE RSQR 0.9999

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	1.01564169	0.00124413	0.9999	0.4614
PH2	1.13453316	0.00096338	0.9999	0.6509
PU	1.52747845	0.00088114	0.9999	1.0103
CONSTANT	2.7674703			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN REGRESSION	3	0.40620E 03	0.40620E 03	
ERROR	8	0.21309E 02	0.71032E 01	0.11873E 0
		0.47859E-04	0.59824E-05	

a = 2.7675
 b = 1.1345
 c = 1.5275
 d = 1.0156

$$K_H = \left(\frac{b}{a}\right) = \left(\frac{1.1345}{2.7675}\right) = 0.4099 \text{ vs } .401$$

$$K_U = \frac{c}{a} = \frac{1.5275}{2.7675} = 0.5519 \text{ vs } 0.552$$

$$K_S = \frac{d}{a} = \frac{1.0156}{2.7675} = 0.3670 \text{ vs } 0.367$$

$$ER = \frac{1}{a^2 K_H K_U} = \frac{1}{(2.7675)^2 (.401)(.552)} = 0.5771 \text{ vs } 0.577$$

NO DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.0026
STANDARD ERROR OF THE MEAN	0.0007
MULTIPLE R	0.9999
MULTIPLE RSQR	0.9999

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.53089857	0.00097763	0.9999	0.3397
PH2	0.70204019	0.00101883	0.9999	0.4276
PU	1.62249946	0.00095471	0.9999	1.0685

CONSTANT 2.7899117

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.34870E 03	0.34870E 03	
REGRESSION	3	0.20882E 02	0.69609E 01	0.97849E
ERROR	9	0.64024E-04	0.71138E-05	

$$a = 2.7899$$

$$K_H = \frac{0.7020}{2.7899} = 0.2516 \quad \text{vs. } 0.250$$

$$b = 0.7020$$

$$K_U = \frac{1.6225}{2.7899} = 0.5816 \quad \text{vs } 0.581$$

$$c = 1.6225$$

$$K_S = \frac{0.5309}{2.7899} = 0.1903 \quad \text{vs } 0.190$$

$$d = 0.5309$$

$$K_R = \frac{1}{a^2 K_H K_U} = 0.8780 \quad \text{vs. } 0.883$$

NO DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.0028
STANDARD ERROR OF THE MEAN	0.0007
MULTIPLE R	0.9999
MULTIPLE RSQR	0.9999

VARIABLE ENTERED PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.06585440	0.00125103	0.9980	0.0378
PH2	0.74263870	0.00095086	0.9999	0.5419
PU	1.64996266	0.00124344	0.9999	0.9755
CONSTANT	3.6588754			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN REGRESSION	1	0.47811E 03	0.47811E 03	0.73493E 0
REGRESSION	3	0.17695E 02	0.58985E 01	
ERROR	11	0.88286E-04	0.80260E-05	

a = 3.6589

$$K_H = \frac{b}{a} = \frac{0.7426}{3.6589} = 0.2030 \quad \text{vs} \quad 0.2030$$

b = 0.7426

$$K_U = \frac{c}{a} = \frac{1.6500}{3.6589} = 0.4509 \quad \text{vs} \quad 0.4510$$

c = 1.6500

$$K_S = \frac{d}{a} = \frac{0.06585}{3.6589} = 0.0180 \quad \text{vs} \quad 0.0180$$

d = 0.06585

$$E_R = \frac{1}{a^2 K_H K_U} = 0.8161 \quad \text{vs} \quad 0.8160$$

```

PAGE 1 11/02/72
// JOB F 1001 2002 3003 4004 F 2
LOG DRIVE CART SPEC CART AVAIL PHY DRIVE
0000 000F 000F 0000
0001 1001 1001 0001
0002 2002 2002 0002
0003 3003 3003 0003
0004 4004 4004 0004

```

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - SYNT GROUP - CSRD

```

// FOR
*ONE WORD INTEGERS
*LIST ALL
*IOCS(CARD,1403 PRINTER)
C HYDROGENATION OF CODIMER
C PROGRAM TO CALC ERROR AFTER FINDING CONSTANTS
C MECHANISM - NO DISSOCIATION OF HYDROGEN
C
REAL KH,KU,KS
DIMENSION PH(20),PU(20),PS(20),REXP(20),RCALC(20),DIFF(20)
C
ICRD=2
LPRT=5
ERROR = 0.0
PHI=0.0
C
*** READ CONSTANTS ***
C
READ(ICRD,100) KH,KU,KS,EK
C
L=0
2 L=L+1
READ(ICRD,102) REXP(L),PH(L),PU(L),PS(L)
IF( PH(L) ) 60,30,20
20 DENOM = 1.+ KH*PH(L) + KU*PU(L) + KS*PS(L)
RCALC(L) = EK*KH*KU*PH(L)*PU(L) / DENOM**2
DIFF(L) = ( REXP(L) - RCALC(L) ) / RCALC(L) * 100.
PHI = PHI + ( RCALC(L) - REXP(L) )**2
GO TO 2
30 KOUNT = L-1
WRITE(LPRT,110)
WRITE(LPRT,111) KH
WRITE(LPRT,112) KU
WRITE(LPRT,113) KS
WRITE(LPRT,114) EK
WRITE(LPRT,120)
DO 50 L = 1,KOUNT
ERROR = ERROR + ABS(DIFF(L))
50 WRITE(LPRT,130) L,RCALC(L),REXP(L),PH(L),PU(L),PS(L),DIFF(L)
XNUM=KOUNT
ERROR = ERROR/XNUM
WRITE(LPRT,140) PHI, ERROR
60 CALL EXIT
C
100 FORMAT( 4F15.0 )
102 FORMAT( 10X,4F10.0 )
110 FORMAT( 1H1 )
111 FORMAT( 6H KH = , F6.4 )
112 FORMAT( 6H KU = , F6.4 )
113 FORMAT( 6H KS = , F6.4 )
114 FORMAT( 6H EK = , F6.4 / )
120 FORMAT( 3X,50H CALC EXPER PH PU PS
1 3X,20H RXN RATE RXN RATE ,35X,10H PCT ERROR )
130 FORMAT( 1X,12,5F10.5,F10.1 )
140 FORMAT( // 18H PHI = , F10.6
1 / 18H AVG PCT ERROR = , F10.1 )
END
VARIABLE ALLOCATIONS
PH(R )=0026-0000 PU(R )=004E-0028 PS(R )=0076-0050 REXP(R
KH(R )=00F0 KU(R )=00F2 KS(R )=00F4 ERROR(R
DENOM(R )=00FC XNUM(R )=00FE ICRD(I )=0104 LPRT(I
STATEMENT ALLOCATIONS
100 =0114 102 =0117 110 =011B 111 =011E 112 =0124 113 =01
2 =01BD 20 =01DC 30 =0229 50 =0264 60 =0294

```

Synthetic Reaction Rates - 15% Error

mech(d) No Dissociation of H_2

200°e

Check error in synthetic data
Should be 15%

KH = 0.4100
KU = 0.5520
KS = 0.3670
EK = 0.5770

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00303	0.00285	0.48200	0.10000	0.50800	-6.0
2	0.02733	0.03006	2.45900	0.52700	0.51500	9.9
3	0.02743	0.03072	2.45000	0.53000	0.51500	11.9
4	0.00534	0.00486	0.47700	0.49400	2.53800	-9.0
5	0.01290	0.01393	0.51400	0.54000	0.45500	7.9
6	0.01219	0.01048	0.47300	0.55200	0.47300	-14.0
7	0.01221	0.01453	0.47000	0.55800	0.47300	18.9
8	0.00332	0.00296	0.10400	0.56200	0.44000	-11.0
9	0.02074	0.02177	0.45000	2.84000	0.23000	4.9
10	0.01880	0.01824	0.40900	2.81000	0.28900	-3.0
11	0.01487	0.00921	0.48400	1.07500	0.94200	-38.0
12	0.01712	0.02483	0.35700	1.59000	0.15300	44.9

PHI = 0.000120
AVG PCT ERROR = 15.0

No Dissociation of H₂

275°C

check error in synthetic data
Should be 15%

KH = 0.2500
KU = 0.5810
KS = 0.1900
EK = 0.8830

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00382	0.00554	0.47800	0.10200	0.52500	44.9
2	0.04071	0.04479	2.50500	0.51800	0.49700	9.9
3	0.04072	0.04398	2.50000	0.51700	0.48500	7.9
4	0.01961	0.01843	0.42500	2.77000	0.31000	-6.0
5	0.02002	0.01722	0.43300	2.80000	0.27000	-14.0
6	0.01657	0.01408	0.48900	0.56200	0.05100	-15.0
7	0.01543	0.00956	0.54600	0.50600	0.44600	-38.0
8	0.01427	0.01593	0.46900	0.55600	0.47500	11.6
9	0.00340	0.00357	0.10000	0.54000	0.46400	4.9
10	0.00714	0.00635	0.42200	0.46200	2.61500	-11.0
11	0.00818	0.00793	0.46700	0.48500	2.55500	-3.0
12	0.03146	0.02863	1.49500	0.51100	0.49500	-9.0
13	0.03856	0.04588	1.22200	0.77600	0.10300	18.9

PHI = 0.000145
AVG PCT ERROR = 14.9

Synthetic Reaction Rates 15% Error
 no dissociation of H₂

100.

KH = 0.2030
 KU = 0.4510
 KS = 0.0180
 EK = 0.8160

325°C

Check error in Synthetic Data
 should be 15%.

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.01866	0.01810	0.50000	2.73500	0.27000	-3.0
2	0.01103	0.01004	0.48200	0.56000	0.06200	-9.0
3	0.01093	0.00940	0.50100	0.53300	0.46600	-14.0
4	0.01069	0.01273	0.47500	0.55300	0.47100	19.0
5	0.01075	0.01559	0.47600	0.55600	0.47800	45.0
6	0.00254	0.00279	0.10100	0.54800	0.45100	9.9
7	0.03194	0.03450	2.33500	0.55000	0.61000	7.9
8	0.02870	0.02296	2.54000	0.45200	0.51000	-20.0
9	0.03128	0.02784	2.40500	0.52400	0.57200	-11.0
10	0.00269	0.00253	0.48900	0.09800	0.51300	-6.0
11	0.00930	0.01042	0.48000	0.48000	2.55000	11.9
12	0.00760	0.00471	0.55500	0.29900	1.64500	-38.0
13	0.01769	0.01592	0.59900	0.99600	0.90700	-9.9
14	0.01576	0.01339	0.43800	1.52300	0.13600	-15.0
15	0.01692	0.01777	0.47800	1.48000	0.14400	4.9

PHI = 0.000101
 AVG PCT ERROR = 15.0

NO DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.6509
STANDARD ERROR OF THE MEAN	0.1878
MULTIPLE R	0.9265
MULTIPLE RSQR	0.8585

VARIABLE ENTERED

PH2

ARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	1.36875844	0.33108860	0.8253	0.5865
PH2	0.93422281	0.25637519	0.7899	0.5055
PU	1.50206685	0.23449021	0.9147	0.9369

NSTANT 2.7533712

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN REGRESSION	1	0.41031E 03	0.41031E 03	0.16183E 0
REGRESSION	3	0.20569E 02	0.68563E 01	
ERROR	8	0.33893E 01	0.42367E 00	

$a = 2.7534$
 $b = 0.9342$
 $c = 1.5021$
 $d = 1.3687$

$$K_H = \frac{b}{a} = \frac{0.9342}{2.7534} = 0.3390$$

$$K_U = \frac{c}{a} = \frac{1.5021}{2.7534} = 0.5455$$

$$K_S = \frac{d}{a} = \frac{1.3687}{2.7534} = 0.4971$$

$$E_k = \frac{1}{a^2 K_H K_U} = 0.7133$$

DISSOCIATION OF HYDROGEN LINEAR REGRESSION

JOB

SUMMARY STATISTICS

NO. OF CASES= 13

VARIABLE		LOW	HIGH	AVERAGE	STD. DEV.
1	RR	0.29649E 01	0.83898E 01	0.52664E 01	0.15067E 01
2	PH2	0.10000E 00	0.25050E 01	0.88853E 00	0.80362E 00
3	PU	0.10200E 00	0.28000E 01	0.85423E 00	0.86877E 00
4	PS	0.51000E-01	0.26150E 01	0.71469E 00	0.84414E 00

NO DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE RR
 RESIDUAL STANDARD DEVIATION 0.4863
 STANDARD ERROR OF THE MEAN 0.1348
 MULTIPLE R 0.9601
 MULTIPLE RSQR 0.9218

VARIABLE ENTERED PH2

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.58964622	0.17827776	0.7406	0.3303
PH2	0.56492984	0.18579182	0.7118	0.3013
PU	1.79352331	0.17409950	0.9601	1.0341
CONSTANT	2.8110380			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN REGRESSION	1	0.36056E 03	0.36056E 03	
REGRESSION	3	0.25112E 02	0.83709E 01	0.35385E 0
ERROR	9	0.21290E 01	0.23656E 00	

2.8110 $K_H = \frac{b}{a} = \frac{0.5649}{2.8110} = 0.2010$

0.5649 $K_U = \frac{c}{a} = \frac{1.7935}{2.8110} = 0.6380$

1.7935 $K_S = \frac{d}{a} = \frac{0.5896}{2.8110} = 0.2097$

0.5896 $E_k = \frac{1}{a^2 K_H K_U} = 0.9869$

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// JOB F 1001 2002 3003 4004 F 2

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - SYNT GROUP - CSRD

```

// FOR
*ONE WORD INTEGERS
*LIST ALL
*IOCS(CARD,1403 PRINTER)
C HYDROGENATION OF CODIMER
C PROGRAM TO CALC ERROR AFTER FINDING CONSTANTS
C MECHANISM - NO DISSOCIATION OF HYDROGEN
C
REAL KH,KU,KS
C DIMENSION PH(20),PU(20),PS(20),REXP(20),RCALC(20),DIFF(20)
C
ICRD=2
LPRT=5
ERROR = 0.0
PHI=0.0
C
*** READ CONSTANTS ***
C
READ(ICRD,100) KH,KU,KS,EK
C
L=0
2 L=L+1
READ(ICRD,102) REXP(L),PH(L),PU(L),PS(L)
IF( PH(L) > 60,30,20
20 DENOM = 1.+ KH*PH(L) + KU*PU(L) + KS*PS(L)
RCALC(L) = EK*KH*KU*PH(L)*PU(L) / DENOM**2
DIFF(L) = ( REXP(L) - RCALC(L) ) / RCALC(L) * 100.
PHI = PHI + ( RCALC(L) - REXP(L) )**2
GO TO 2
30 KOUNT = L-1
WRITE(LPRT,110)
WRITE(LPRT,111) KH
WRITE(LPRT,112) KU
WRITE(LPRT,113) KS
WRITE(LPRT,114) EK
WRITE(LPRT,120)
DO 50 L = 1,KOUNT
ERROR = ERROR + ABS(DIFF(L))
50 WRITE(LPRT,130) L,RCALC(L),REXP(L),PH(L),PU(L),PS(L),DIFF(L)
XNUM=XNUM+1
ERROR = ERROR/XNUM
WRITE(LPRT,140) PHI, ERROR
60 CALL EXIT
C
100 FORMAT( 4F15.0 )
102 FORMAT( 10X,4F10.0 )
110 FORMAT( 1H1 )
111 FORMAT( 6H KH = , F6.4 )
112 FORMAT( 6H KU = , F6.4 )
113 FORMAT( 6H KS = , F6.4 )
114 FORMAT( 6H EK = , F6.4 / )
120 FORMAT( 3X,50H CALC EXPER PH PU PS /
1 3X,20H RXN RATE RXN RATE ,35X,10H PCT ERROR )
130 FORMAT( 1X,12,5F10.5,F10.1 )
140 FORMAT( // 18H PHI = , F10.6
1 / 18H AVG PCT ERROR = , F10.1 )
END
VARIABLE ALLOCATIONS
PH(R )=0026-0000 PU(R )=004E-0028 PS(R )=0076-0050 REXP(R )=(
KH(R )=00F0 KU(R )=00F2 KS(R )=00F4 ERROR(R )=(
DENOM(R )=00FC XNUM(R )=00FE ICRD(I )=0104 LPRT(I )=(
STATEMENT ALLOCATIONS
100 =0114 102 =0117 110 =011B 111 =011E 112 =0124 113 =012A
2 =018D 20 =01DC 30 =0229 50 =0264 60 =0294

```

~~Hydrolysis~~ mechanism (d) - Results of linear regression

200°C

KH = 0.3390
 KU = 0.5450
 KS = 0.4970
 EK = 0.7130

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00293	0.00285	0.48200	0.10000	0.50800	-2.7
2	0.03021	0.03006	2.45900	0.52700	0.51500	-0.4
3	0.03031	0.03072	2.45000	0.53000	0.51500	1.3
4	0.00428	0.00486	0.47700	0.49400	2.53800	13.5
5	0.01273	0.01393	0.51400	0.54000	0.45500	9.4
6	0.01195	0.01048	0.47300	0.55200	0.47300	-12.2
7	0.01197	0.01453	0.47000	0.55800	0.47300	21.3
8	0.00316	0.00296	0.10400	0.56200	0.44000	-6.3
9	0.02125	0.02177	0.45000	2.84000	0.23000	2.4
10	0.01912	0.01824	0.40900	2.81000	0.28900	-4.6
11	0.01393	0.00921	0.48400	1.07500	0.94200	-33.8
12	0.01755	0.02483	0.35700	1.59000	0.15300	41.4

PHI. = 0.000086
 AVG PCT ERROR = 12.5

Synthetic Reaction Paths with 15% Error

Mechanism (d) - Results of Linear Regression

107.

KH = 0.2010
KU = 0.6380
KS = 0.2100
EK = 0.9870

275°C

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00381	0.00554	0.47800	0.10200	0.52500	45.2
2	0.04371	0.04479	2.50500	0.51800	0.49700	2.4
3	0.04372	0.04398	2.50000	0.51700	0.48500	0.5
4	0.01750	0.01843	0.42500	2.77000	0.31000	5.3
5	0.01787	0.01722	0.43300	2.80000	0.27000	-3.6
6	0.01615	0.01408	0.48900	0.56200	0.05100	-12.7
7	0.01501	0.00956	0.54600	0.50600	0.44600	-36.2
8	0.01376	0.01593	0.46900	0.55600	0.47500	15.7
9	0.00319	0.00357	0.10000	0.54000	0.46400	11.6
10	0.00663	0.00635	0.42200	0.46200	2.61500	-4.1
11	0.00761	0.00793	0.46700	0.48500	2.55500	4.1
12	0.03229	0.02863	1.49500	0.51100	0.49500	-11.3
13	0.03864	0.04588	1.22200	0.77600	0.10300	18.7

PHI = 0.000110
AVG PCT ERROR = 13.2

Mechanism (d) - Results of Linear Regression

325°C

KH = 0.2510
 KU = 0.4790
 KS = 0.0480
 EK = 0.6590

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.01807	0.01810	0.50000	2.73500	0.27000	0.1
2	0.01103	0.01004	0.48200	0.56000	0.06200	-8.9
3	0.01074	0.00940	0.50100	0.53300	0.46600	-12.4
4	0.01051	0.01273	0.47500	0.55300	0.47100	21.0
5	0.01056	0.01559	0.47600	0.55600	0.47800	47.5
6	0.00255	0.00279	0.10100	0.54800	0.45100	9.2
7	0.02882	0.03450	2.33500	0.55000	0.61000	19.6
8	0.02577	0.02296	2.54000	0.45200	0.51000	-10.9
9	0.02818	0.02784	2.40500	0.52400	0.57200	-1.2
10	0.00266	0.00253	0.48900	0.09800	0.51300	-4.8
11	0.00841	0.01042	0.48000	0.48000	2.55000	23.8
12	0.00709	0.00471	0.55500	0.29900	1.64500	-33.5
13	0.01692	0.01592	0.59900	0.99600	0.90700	-5.9
14	0.01551	0.01339	0.43800	1.52300	0.13600	-13.6
15	0.01663	0.01777	0.47800	1.48000	0.14400	6.8

PHI = 0.000089
 AVG PCT ERROR = 14.6


```

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// JOB F 1001 2002 3003 4004 F 2002
LOG DRIVE CART SPEC CART AVAIL PHY DRIVE
0000 000F 000F 0000
0001 1001 1001 0001
0002 2002 2002 0002
0003 3003 3003 0003
0004 4004 4004 0004

```

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - LSEST GROUP - CSRD

```

// FOR
*ONE WORD INTEGERS
*LIST ALL
SUBROUTINE FUN(BB)
DIMENSION BB(10)
COMMON KEY,MJM,ND,NF,NFD,NI,NP,PHIZ,SL,B(10),F( 40),G(10),S(10),
1 Y( 40),A(10,10),X(40,16),P(1,10),IPRIN,ILM,MAT,MAR,IPART,
2 FF( 40),KPOIN,NR,NW
DO 1 I=1,ND
DENOM=(1+BB(1)*X(I,1)+BB(2)*X(I,2)+BB(3)*X(I,3))
1 FF(I) = BB(1)*BB(2)*BB(4)*X(I,1)*X(I,2) / DENOM**2
RETURN
END

```

```

VARIABLE ALLOCATIONS
KEY(IC)=7FFF MJM(IC)=7FFE ND(IC)=7FFD NF(IC)=7FFC
NP(IC)=7FF9 PHIZ(RC)=7FF6 SL(RC)=7FF4 B(RC)=7FF2
S(RC)=7F7A-7F68 Y(RC)=7F66-7F18 A(RC)=7F16-7E50 X(RC)=7E4E
ILM(IC)=793A MAT(IC)=7939 MAR(IC)=7938 IPART(IC)=7937
NR(IC)=78E4 NW(IC)=78E3 DENOM(R )=0000 I(I )=0008

```

```

STATEMENT ALLOCATIONS
1 =C058

```

FEATURES SUPPORTED ONE WORD INTEGERS

```

CALLED SUBPROGRAMS
FADD FMPYX FLD FLDX FSTO FSTOX FDVR FAXI FLOAT SU

```

```

INTEGER CONSTANTS
1=0010 2=0011

```

```

CORE REQUIREMENTS FOR FUN
COMMON 1822 VARIABLES 16 PROGRAM 116

```

RELATIVE ENTRY POINT ADDRESS IS 0012 (HEX)

END OF COMPILATION

// DUP

```

*DELETE FUN 2002
CART ID 2002 DB ADDR 3BF1 DB CNT 000A

```

```

*STORE WS UA FUN 2002 2002
CART ID 2002 DB ADDR 3F7B DB CNT 0009

```

// JOB F 1001 2002 3003 4004 F 2002

PAP

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - LSEST GROUP - CSRD

// FOR

*ONE WORD INTEGERS

*LIST ALL

```

SUBROUTINE PART
COMMON KEY, MJM, ND, NF, NFD, NI, NP, PHIZ, SL, B(10), F( 40), G(10), S(10),
1 Y( 40), A(10,10), X(40,16), P(1,10), IPRIN, ILM, MAT, MAR, IPART,
2 FF( 40), KPOIN, NR, NW
K=KPOIN
DENOM=(1+ B(1)*X(K,1)+ B(2)*X(K,2)+ B(3)*X(K,3))
P(1,1)= B(2)*B(4)*X(K,1)*X(K,2)*(DENOM-2*B(1)*X(K,1)) / DENOM**3
P(1,2)= B(1)*B(4)*X(K,1)*X(K,2)*(DENOM-2*B(2)*X(K,2)) / DENOM**3
P(1,3)= 2.0*B(1)*B(2)*B(4)*X(K,1)*X(K,2)*X(K,3) /DENOM**3
P(1,4)= B(1)*B(2)*X(K,1)*X(K,2) / DENOM**2
RETURN
END

```

VARIABLE ALLOCATIONS

KEY(IC)=7FFF	MJM(IC)=7FFE	ND(IC)=7FFD	NF(IC)=7FFC
NP(IC)=7FF9	PHIZ(RC)=7FF6	SL(RC)=7FF4	B(RC)=7FF2
S(RC)=7F7A-7F68	Y(RC)=7F66-7F18	A(RC)=7F16-7E50	X(RC)=7E4E
ILM(IC)=793A	MAT(IC)=7939	MAR(IC)=7938	IPART(IC)=7937
NR(IC)=78E4	NW(IC)=78E3	DENOM(R)=0000	K(I)=0008

FEATURES SUPPORTED
ONE WORD INTEGERS

CALLED SUBPROGRAMS									
FADD	FMPY	FMPYX	FLD	FLOX	FSTO	FSTOX	FSBR	FDVR	FA

REAL CONSTANTS
.200000E 01=0010

INTEGER CONSTANTS
1=0012 2=0013 3=0014

CORE REQUIREMENTS FOR PART
COMMON 1822 VARIABLES 16 PROGRAM 224

RELATIVE ENTRY POINT ADDRESS IS 0015 (HEX)

END OF COMPILATION

// DUP

*DELETE	PART	2002
CART ID 2002	DB ADDR 3BF1	DB CNT 0012

*STORE	WS	UA	PART	2002	2002
CART ID 2002	DB ADDR 3F74	DB CNT 0012			

Synthetic Data with 12% error - Parameters from linear regression
 No dissociation - ros'c

111.

DEPENDENT	INDEPENDENT	2	3
	1		
0.28550E-02	0.48200E 00	0.10000E 00	0.50800E 00
0.30068E-01	0.24590E 01	0.52700E 00	0.51500E 00
0.30727E-01	0.24500E 01	0.53000E 00	0.51500E 00
0.48620E-02	0.47700E 00	0.49400E 00	0.25380E 00
0.13938E-01	0.51400E 00	0.54000E 00	0.45500E 00
0.10485E-01	0.47300E 00	0.55200E 00	0.47300E 00
0.14537E-01	0.47000E 00	0.55800E 00	0.47300E 00
0.29620E-02	0.10400E 00	0.56200E 00	0.44000E 00
0.21778E-01	0.45000E 00	0.28400E 01	0.23000E 00
0.18243E-01	0.40900E 00	0.28100E 01	0.28900E 00
0.92190E-02	0.48400E 00	0.10750E 01	0.94200E 00
0.24837E-01	0.35700E 00	0.15900E 01	0.15300E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.86975E-04 PARAMETERS	SQRT(PHI)/ND= 0.77717E-03 0.33900E 00 0.54500E 00	LAMBDA= 0.10000E-01 0.49700E 00 0.71300E 00
PHI= 0.86066E-04 PARAMETERS	SQRT(PHI)/ND= 0.77309E-03 0.34052E 00 0.54540E 00	LAMBDA= 0.10000E 02 0.49416E 00 0.71456E 00
PHI= 0.85640E-04 PARAMETERS	SQRT(PHI)/ND= 0.77118E-03 0.34180E 00 0.54550E 00	LAMBDA= 0.99999E 01 0.49037E 00 0.71578E 00
PHI= 0.85586E-04 PARAMETERS	SQRT(PHI)/ND= 0.77093E-03 0.34287E 00 0.54532E 00	LAMBDA= 0.99999E 01 0.48575E 00 0.71670E 00
PHI= 0.85578E-04 PARAMETERS	SQRT(PHI)/ND= 0.77090E-03 0.34290E 00 0.54532E 00	LAMBDA= 0.99999E-01 0.48575E 00 0.71670E 00
PHI= 0.85570E-04 PARAMETERS	SQRT(PHI)/ND= 0.77086E-03 0.34293E 00 0.54532E 00	LAMBDA= 0.99999E-01 0.48576E 00 0.71670E 00
PHI= 0.85562E-04 PARAMETERS	SQRT(PHI)/ND= 0.77083E-03 0.34296E 00 0.54533E 00	LAMBDA= 0.99999E-01 0.48577E 00 0.71670E 00
PHI= 0.85554E-04 PARAMETERS	SQRT(PHI)/ND= 0.77079E-03 0.34300E 00 0.54533E 00	LAMBDA= 0.99999E-01 0.48577E 00 0.71670E 00
PHI= 0.85546E-04 PARAMETERS	SQRT(PHI)/ND= 0.77076E-03 0.34303E 00 0.54534E 00	LAMBDA= 0.99999E-01 0.48578E 00 0.71670E 00
PHI= 0.85539E-04 PARAMETERS	SQRT(PHI)/ND= 0.77072E-03 0.34306E 00 0.54534E 00	LAMBDA= 0.99999E-01 0.48578E 00 0.71670E 00
PHI= 0.85531E-04 PARAMETERS	SQRT(PHI)/ND= 0.77069E-03 0.34309E 00 0.54535E 00	LAMBDA= 0.99999E-01 0.48579E 00 0.71670E 00
PHI= 0.85524E-04 PARAMETERS	SQRT(PHI)/ND= 0.77066E-03 0.34312E 00 0.54535E 00	LAMBDA= 0.99999E-01 0.48579E 00 0.71670E 00
PHI= 0.85516E-04 PARAMETERS	SQRT(PHI)/ND= 0.77062E-03 0.34315E 00 0.54536E 00	LAMBDA= 0.99999E-01 0.48580E 00 0.71670E 00
PHI= 0.85509E-04 PARAMETERS	SQRT(PHI)/ND= 0.77059E-03 0.34318E 00 0.54536E 00	LAMBDA= 0.99999E-01 0.48581E 00 0.71670E 00
PHI= 0.85501E-04 PARAMETERS	SQRT(PHI)/ND= 0.77056E-03 0.34322E 00 0.54536E 00	LAMBDA= 0.99999E-01 0.48581E 00 0.71670E 00
PHI= 0.85494E-04 PARAMETERS	SQRT(PHI)/ND= 0.77052E-03 0.34325E 00 0.54537E 00	LAMBDA= 0.99999E-01 0.48582E 00 0.71670E 00
PHI= 0.85487E-04 PARAMETERS	SQRT(PHI)/ND= 0.77049E-03 0.34328E 00 0.54537E 00	LAMBDA= 0.99999E-01 0.48582E 00 0.71670E 00
PHI= 0.85480E-04 PARAMETERS	SQRT(PHI)/ND= 0.77046E-03 0.34331E 00 0.54538E 00	LAMBDA= 0.99999E-01 0.48583E 00 0.71670E 00
PHI= 0.85473E-04 PARAMETERS	SQRT(PHI)/ND= 0.77043E-03 0.34334E 00 0.54538E 00	LAMBDA= 0.99999E-01 0.48584E 00 0.71670E 00
PHI= 0.85466E-04 PARAMETERS	SQRT(PHI)/ND= 0.77039E-03 0.34337E 00 0.54539E 00	LAMBDA= 0.99999E-01 0.48584E 00 0.71670E 00

PHI= 0.85458E-04 PARAMETERS	SQRT(PHI)/ND= 0.77036E-03 0.34340E 00 0.54539E 00	LAMBDA= 0.99999E-01 0.48585E 00 0.71670E 00
PHI= 0.85451E-04 PARAMETERS	SQRT(PHI)/ND= 0.77033E-03 0.34343E 00 0.54540E 00	LAMBDA= 0.99999E-01 0.48585E 00 0.71670E 00
PHI= 0.85445E-04 PARAMETERS	SQRT(PHI)/ND= 0.77030E-03 0.34346E 00 0.54540E 00	LAMBDA= 0.99999E-01 0.48586E 00 0.71669E 00
PHI= 0.85438E-04 PARAMETERS	SQRT(PHI)/ND= 0.77027E-03 0.34349E 00 0.54541E 00	LAMBDA= 0.99999E-01 0.48586E 00 0.71669E 00
PHI= 0.85431E-04 PARAMETERS	SQRT(PHI)/ND= 0.77024E-03 0.34352E 00 0.54541E 00	LAMBDA= 0.99999E-01 0.48587E 00 0.71669E 00
PHI= 0.85424E-04 PARAMETERS	SQRT(PHI)/ND= 0.77021E-03 0.34355E 00 0.54541E 00	LAMBDA= 0.99999E-01 0.48588E 00 0.71669E 00
PHI= 0.85417E-04 PARAMETERS	SQRT(PHI)/ND= 0.77018E-03 0.34358E 00 0.54542E 00	LAMBDA= 0.99999E-01 0.48588E 00 0.71669E 00
PHI= 0.85410E-04 PARAMETERS	SQRT(PHI)/ND= 0.77015E-03 0.34361E 00 0.54542E 00	LAMBDA= 0.99999E-01 0.48589E 00 0.71669E 00
PHI= 0.85404E-04 PARAMETERS	SQRT(PHI)/ND= 0.77012E-03 0.34364E 00 0.54543E 00	LAMBDA= 0.99999E-01 0.48589E 00 0.71669E 00

ALGORITHM TERMINATED

PHI= 0.85404E-04 PARAMETERS	SQRT(PHI)/ND= 0.77012E-03 0.34364E 00 0.54543E 00	LAMBDA= 0.99999E 04 0.48589E 00 0.71669E 00
--------------------------------	--	--

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3
		1		
0.30085E-02	-0.15358E-03	0.48200E 00	0.10000E 00	0.50800E 00
0.30663E-01	-0.59508E-03	0.24590E 01	0.52700E 00	0.51500E 00
0.30762E-01	-0.35386E-04	0.24500E 01	0.53000E 00	0.51500E 00
0.44516E-02	0.41033E-03	0.47700E 00	0.49400E 00	0.25380E 00
0.13020E-01	0.91798E-03	0.51400E 00	0.54000E 00	0.45500E 00
0.12230E-01	-0.17453E-02	0.47300E 00	0.55200E 00	0.47300E 00
0.12252E-01	0.22846E-02	0.47000E 00	0.55800E 00	0.47300E 00
0.32426E-02	-0.28062E-03	0.10400E 00	0.56200E 00	0.44000E 00
0.21658E-01	0.11961E-03	0.45000E 00	0.28400E 01	0.23000E 00
0.19501E-01	-0.12588E-02	0.40900E 00	0.28100E 01	0.28900E 00
0.14305E-01	-0.50865E-02	0.48400E 00	0.10750E 01	0.94200E 00
0.17894E-01	0.69425E-02	0.35700E 00	0.15900E 01	0.15300E 00

CORRELATION MATRIX

1.000			
0.506	1.000		
0.749	0.883	1.000	
0.895	0.806	0.887	1.000

29 STEPS

no dissociation of H₂ - 275°C

(13)

DEPENDENT	INDEPENDENT	2	3
	1		
0.55460E-02	0.47800E 00	0.10200E 00	0.52500E
0.44790E-01	0.25050E 01	0.51800E 00	0.49700E
0.43983E-01	0.25000E 01	0.51700E 00	0.48500E
0.18437E-01	0.42500E 00	0.27700E 01	0.31000E
0.17224E-01	0.43300E 00	0.28000E 01	0.27000E
0.14084E-01	0.48900E 00	0.56200E 00	0.51000E
0.95680E-02	0.54600E 00	0.50600E 00	0.44600E
0.15934E-01	0.46900E 00	0.55600E 00	0.47500E
0.35710E-02	0.10000E 00	0.54000E 00	0.46400E
0.63580E-02	0.42200E 00	0.46200E 00	0.26150E
0.79380E-02	0.46700E 00	0.48500E 00	0.25550E
0.28631E-01	0.14950E 01	0.51100E 00	0.49500E
0.45888E-01	0.12220E 01	0.77600E 00	0.10300E

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 LS A + SL*D-1

PHI= 0.11031E-03 PARAMETERS	SQRT(PHI)/ND= 0.80794E-03 0.20100E 00 0.63800E 00	LAMBDA= 0.10000E-01 0.21000E 00 0.98700E
PHI= 0.10954E-03 PARAMETERS	SQRT(PHI)/ND= 0.80511E-03 0.20147E 00 0.63880E 00	LAMBDA= 0.10000E 02 0.20836E 00 0.98857E
PHI= 0.10927E-03 PARAMETERS	SQRT(PHI)/ND= 0.80410E-03 0.20184E 00 0.63926E 00	LAMBDA= 0.99999E 01 0.20620E 00 0.98982E
PHI= 0.10927E-03 PARAMETERS	SQRT(PHI)/ND= 0.80409E-03 0.20187E 00 0.63929E 00	LAMBDA= 0.99999E 02 0.20594E 00 0.98992E
PHI= 0.10855E-03 PARAMETERS	SQRT(PHI)/ND= 0.80145E-03 0.20390E 00 0.63970E 00	LAMBDA= 0.99999E-01 0.20617E 00 0.99047E
PHI= 0.10850E-03 PARAMETERS	SQRT(PHI)/ND= 0.80127E-03 0.20442E 00 0.63981E 00	LAMBDA= 0.99999E-01 0.20623E 00 0.99061E
PHI= 0.10849E-03 PARAMETERS	SQRT(PHI)/ND= 0.80125E-03 0.20455E 00 0.63983E 00	LAMBDA= 0.99999E-01 0.20625E 00 0.99065E
PHI= 0.10849E-03 PARAMETERS	SQRT(PHI)/ND= 0.80125E-03 0.20465E 00 0.63986E 00	LAMBDA= 0.99999E-01 0.20626E 00 0.99068E
PHI= 0.10823E-03 PARAMETERS	SQRT(PHI)/ND= 0.80028E-03 0.20464E 00 0.63986E 00	LAMBDA= 0.99999E 01 0.20769E 00 0.99066E
PHI= 0.10823E-03 PARAMETERS	SQRT(PHI)/ND= 0.80027E-03 0.20474E 00 0.63988E 00	LAMBDA= 0.99999E-01 0.20770E 00 0.99069E
PHI= 0.10823E-03 PARAMETERS	SQRT(PHI)/ND= 0.80027E-03 0.20480E 00 0.63990E 00	LAMBDA= 0.99999E-01 0.20771E 00 0.99071E
PHI= 0.10797E-03 PARAMETERS	SQRT(PHI)/ND= 0.79933E-03 0.20480E 00 0.63990E 00	LAMBDA= 0.99999E 01 0.20910E 00 0.99069E
PHI= 0.10797E-03 PARAMETERS	SQRT(PHI)/ND= 0.79932E-03 0.20507E 00 0.63996E 00	LAMBDA= 0.99999E-01 0.20914E 00 0.99077E
PHI= 0.10797E-03 PARAMETERS	SQRT(PHI)/ND= 0.79932E-03 0.20497E 00 0.63994E 00	LAMBDA= 0.99999E-01 0.20913E 00 0.99074E
PHI= 0.10797E-03 PARAMETERS	SQRT(PHI)/ND= 0.79932E-03 0.20494E 00 0.63993E 00	LAMBDA= 0.99999E-01 0.20912E 00 0.99073E
PHI= 0.10773E-03 PARAMETERS	SQRT(PHI)/ND= 0.79842E-03 0.20494E 00 0.63993E 00	LAMBDA= 0.99999E 01 0.21049E 00 0.99071E
PHI= 0.10772E-03 PARAMETERS	SQRT(PHI)/ND= 0.79840E-03 0.20506E 00 0.63996E 00	LAMBDA= 0.99999E-01 0.21050E 00 0.99074E
PHI= 0.10772E-03 PARAMETERS	SQRT(PHI)/ND= 0.79840E-03 0.20515E 00 0.63998E 00	LAMBDA= 0.99999E-01 0.21051E 00 0.99077E
PHI= 0.10749E-03 PARAMETERS	SQRT(PHI)/ND= 0.79752E-03 0.20514E 00 0.63997E 00	LAMBDA= 0.99999E 01 0.21186E 00 0.99074E
PHI= 0.10748E-03	SQRT(PHI)/ND= 0.79751E-03	LAMBDA= 0.99999E-01

PARAMETERS	0.20539E 00	0.64003E 00	0.21189E 00	0.99082E
PHI= 0.10748E-03	SQRT(PHI)/ND= 0.79751E-03		LAMBDA= 0.99999E-01	
PARAMETERS	0.20530E 00	0.64001E 00	0.21188E 00	0.99079E
PHI= 0.10726E-03	SQRT(PHI)/ND= 0.79666E-03		LAMBDA= 0.99999E 01	
PARAMETERS	0.20529E 00	0.64001E 00	0.21320E 00	0.99077E
PHI= 0.10725E-03	SQRT(PHI)/ND= 0.79665E-03		LAMBDA= 0.99999E-01	
PARAMETERS	0.20556E 00	0.64007E 00	0.21323E 00	0.99085E
PHI= 0.10725E-03	SQRT(PHI)/ND= 0.79665E-03		LAMBDA= 0.99999E-01	
PARAMETERS	0.20546E 00	0.64005E 00	0.21322E 00	0.99082E
PHI= 0.10703E-03	SQRT(PHI)/ND= 0.79583E-03		LAMBDA= 0.99999E 01	
PARAMETERS	0.20546E 00	0.64004E 00	0.21452E 00	0.99079E
PHI= 0.10703E-03	SQRT(PHI)/ND= 0.79582E-03		LAMBDA= 0.99999E-01	
PARAMETERS	0.20571E 00	0.64010E 00	0.21455E 00	0.99087E
PHI= 0.10703E-03	SQRT(PHI)/ND= 0.79582E-03		LAMBDA= 0.99999E-01	
PARAMETERS	0.20561E 00	0.64008E 00	0.21454E 00	0.99084E
PHI= 0.10703E-03	SQRT(PHI)/ND= 0.79582E-03		LAMBDA= 0.99999E-01	
PARAMETERS	0.20559E 00	0.64008E 00	0.21453E 00	0.99084E
PHI= 0.10682E-03	SQRT(PHI)/ND= 0.79503E-03		LAMBDA= 0.99999E 01	
PARAMETERS	0.20559E 00	0.64007E 00	0.21580E 00	0.99080E

ALGORITHM TERMINATED

PHI= 0.10682E-03	SQRT(PHI)/ND= 0.79503E-03		LAMBDA= 0.99999E 04	
PARAMETERS	0.20559E 00	0.64007E 00	0.21580E 00	0.99080E

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3
		1		
0.38991E-02	0.16468E-02	0.47800E 00	0.10200E 00	0.52500E
0.44319E-01	0.47051E-03	0.25050E 01	0.51800E 00	0.49700E
0.44338E-01	-0.35566E-03	0.25000E 01	0.51700E 00	0.48500E
0.17912E-01	0.52412E-03	0.42500E 00	0.27700E 01	0.31000E
0.18294E-01	-0.10707E-02	0.43300E 00	0.28000E 01	0.27000E
0.16553E-01	-0.24695E-02	0.48900E 00	0.56200E 00	0.51000E-
0.15340E-01	-0.57724E-02	0.54600E 00	0.50600E 00	0.44600E
0.14064E-01	0.18696E-02	0.46900E 00	0.55600E 00	0.47500E
0.32745E-02	0.29642E-03	0.10000E 00	0.54000E 00	0.46400E
0.67071E-02	-0.34912E-03	0.42200E 00	0.46200E 00	0.26150E
0.77043E-02	0.23366E-03	0.46700E 00	0.48500E 00	0.25550E
0.32851E-01	-0.42209E-02	0.14950E 01	0.51100E 00	0.49500E
0.39458E-01	0.64299E-02	0.12220E 01	0.77600E 00	0.10300E

CORRELATION MATRIX

1.000			
0.804	1.000		
0.755	0.838	1.000	
0.966	0.912	0.808	1.000

29 STEPS

No dissociation - 325°C

DEPENDENT	INDEPENDENT		2	3
	1			
0.18100E-01	0.50000E 00	0.27350E 01	0.27000E	
0.10045E-01	0.48200E 00	0.56000E 00	0.62000E	
0.94070E-02	0.50100E 00	0.53300E 00	0.46600E	
0.12732E-01	0.47500E 00	0.55300E 00	0.47100E	
0.15592E-01	0.47600E 00	0.55600E 00	0.47800E	
0.27940E-02	0.10100E 00	0.54800E 00	0.45100E	
0.34500E-01	0.23350E 01	0.55000E 00	0.61000E	
0.22962E-01	0.25400E 01	0.45200E 00	0.51000E	
0.27840E-01	0.24050E 01	0.52400E 00	0.57200E	
0.25320E-02	0.48900E 00	0.98000E-01	0.51300E	
0.10425E-01	0.48000E 00	0.48000E 00	0.25500E	
0.47120E-02	0.55500E 00	0.29900E 00	0.16450E	
0.15925E-01	0.59900E 00	0.99600E 00	0.90700E	
0.13396E-01	0.43800E 00	0.15230E 01	0.13600E	
0.17770E-01	0.47800E 00	0.14800E 01	0.14400E	

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.89725E-04 PARAMETERS	SQRT(PHI)/ND= 0.63149E-03 0.25100E 00	0.47900E 00	LAMBDA= 0.10000E-01 0.48000E-01	0.65900E
PHI= 0.89341E-04 PARAMETERS	SQRT(PHI)/ND= 0.63013E-03 0.25190E 00	0.48525E 00	LAMBDA= 0.10000E 01 0.60721E-01	0.66169E
PHI= 0.89239E-04 PARAMETERS	SQRT(PHI)/ND= 0.62977E-03 0.25234E 00	0.48667E 00	LAMBDA= 0.10000E 02 0.63869E-01	0.66259E
PHI= 0.89236E-04 PARAMETERS	SQRT(PHI)/ND= 0.62976E-03 0.25273E 00	0.48797E 00	LAMBDA= 0.99999E 01 0.66966E-01	0.66337E
PHI= 0.89236E-04 PARAMETERS	SQRT(PHI)/ND= 0.62976E-03 0.25278E 00	0.48812E 00	LAMBDA= 0.99999E 02 0.67330E-01	0.66347E
PHI= 0.89236E-04 PARAMETERS	SQRT(PHI)/ND= 0.62976E-03 0.25278E 00	0.48814E 00	LAMBDA= 0.99999E 03 0.67367E-01	0.66348E
PHI= 0.89235E-04 PARAMETERS	SQRT(PHI)/ND= 0.62976E-03 0.25278E 00	0.48814E 00	LAMBDA= 0.99999E 02 0.67368E-01	0.66348E
PHI= 0.89230E-04 PARAMETERS	SQRT(PHI)/ND= 0.62974E-03 0.25280E 00	0.48815E 00	LAMBDA= 0.99999E 01 0.67377E-01	0.66349E
PHI= 0.89177E-04 PARAMETERS	SQRT(PHI)/ND= 0.62955E-03 0.25292E 00	0.48826E 00	LAMBDA= 0.99999E 00 0.67463E-01	0.66358E
PHI= 0.88865E-04 PARAMETERS	SQRT(PHI)/ND= 0.62845E-03 0.25372E 00	0.48910E 00	LAMBDA= 0.99999E-01 0.68214E-01	0.66423E
PHI= 0.88699E-04 PARAMETERS	SQRT(PHI)/ND= 0.62786E-03 0.25429E 00	0.48983E 00	LAMBDA= 0.99999E-01 0.68912E-01	0.66473E
PHI= 0.88614E-04 PARAMETERS	SQRT(PHI)/ND= 0.62756E-03 0.25468E 00	0.49048E 00	LAMBDA= 0.99999E-01 0.69571E-01	0.66512E
PHI= 0.88576E-04 PARAMETERS	SQRT(PHI)/ND= 0.62743E-03 0.25495E 00	0.49107E 00	LAMBDA= 0.99999E-01 0.70202E-01	0.66543E
PHI= 0.88564E-04 PARAMETERS	SQRT(PHI)/ND= 0.62738E-03 0.25513E 00	0.49161E 00	LAMBDA= 0.99999E-01 0.70811E-01	0.66568E
PHI= 0.88563E-04 PARAMETERS	SQRT(PHI)/ND= 0.62738E-03 0.25515E 00	0.49166E 00	LAMBDA= 0.99999E 00 0.70874E-01	0.66570E
PHI= 0.88562E-04 PARAMETERS	SQRT(PHI)/ND= 0.62738E-03 0.25517E 00	0.49172E 00	LAMBDA= 0.99999E 00 0.70937E-01	0.66573E
PHI= 0.88561E-04 PARAMETERS	SQRT(PHI)/ND= 0.62738E-03 0.25519E 00	0.49178E 00	LAMBDA= 0.99999E 00 0.70999E-01	0.66576E
PHI= 0.88561E-04 PARAMETERS	SQRT(PHI)/ND= 0.62737E-03 0.25521E 00	0.49183E 00	LAMBDA= 0.99999E 00 0.71062E-01	0.66578E
PHI= 0.88560E-04 PARAMETERS	SQRT(PHI)/ND= 0.62737E-03 0.25523E 00	0.49189E 00	LAMBDA= 0.99999E 00 0.71124E-01	0.66581E

PHI= 0.88560E-04 PARAMETERS	SQRT(PHI)/ND= 0.62737E-03 0.25525E 00	0.49194E 00	LAMBDA= 0.99999E 00 0.71186E-01	0.66583E
PHI= 0.88560E-04 PARAMETERS	SQRT(PHI)/ND= 0.62737E-03 0.25525E 00	0.49194E 00	LAMBDA= 0.99999E 01 0.71192E-01	0.66583E
PHI= 0.88560E-04 PARAMETERS	SQRT(PHI)/ND= 0.62737E-03 0.25525E 00	0.49195E 00	LAMBDA= 0.99999E 01 0.71199E-01	0.66584E
PHI= 0.88534E-04 PARAMETERS	SQRT(PHI)/ND= 0.62728E-03 0.25626E 00	0.49231E 00	LAMBDA= 0.99999E-01 0.71417E-01	0.66640E
PHI= 0.88531E-04 PARAMETERS	SQRT(PHI)/ND= 0.62727E-03 0.25610E 00	0.49227E 00	LAMBDA= 0.99999E-01 0.71393E-01	0.66634E
PHI= 0.88531E-04 PARAMETERS	SQRT(PHI)/ND= 0.62727E-03 0.25610E 00	0.49227E 00	LAMBDA= 0.99999E 02 0.71393E-01	0.66634E
PHI= 0.88531E-04 PARAMETERS	SQRT(PHI)/ND= 0.62727E-03 0.25610E 00	0.49227E 00	LAMBDA= 0.99999E 02 0.71394E-01	0.66634E

ALGORITHM CONVERGED

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3
		1		
0.18474E-01	-0.37405E-03	0.50000E 00	0.27350E 01	0.27000E
0.11510E-01	-0.14658E-02	0.48200E 00	0.56000E 00	0.62000E-
0.11063E-01	-0.16565E-02	0.50100E 00	0.53300E 00	0.46600E
0.10828E-01	0.19030E-02	0.47500E 00	0.55300E 00	0.47100E
0.10876E-01	0.47153E-02	0.47600E 00	0.55600E 00	0.47800E
0.26371E-02	0.15681E-03	0.10100E 00	0.54800E 00	0.45100E
0.29502E-01	0.49975E-02	0.23350E 01	0.55000E 00	0.61000E
0.26453E-01	-0.34919E-02	0.25400E 01	0.45200E 00	0.51000E
0.28877E-01	-0.10374E-02	0.24050E 01	0.52400E 00	0.57200E
0.27492E-02	-0.21725E-03	0.48900E 00	0.98000E-01	0.51300E
0.81478E-02	0.22771E-02	0.48000E 00	0.48000E 00	0.25500E
0.70443E-02	-0.23323E-02	0.55500E 00	0.29900E 00	0.16450E
0.17171E-01	-0.12460E-02	0.59900E 00	0.99600E 00	0.90700E
0.15997E-01	-0.26019E-02	0.43800E 00	0.15230E 01	0.13600E
0.17155E-01	0.61476E-03	0.47800E 00	0.14800E 01	0.14400E

CORRELATION MATRIX

1.000			
0.693	1.000		
0.710	0.809	1.000	
0.915	0.905	0.787	1.000

25 STEPS


```
PAGE 1      02/06/73
// JOB      F 1001 2002 3003 4004      F 2
LOG DRIVE   CART SPEC      CART AVAIL  PHY DRIVE
0000        000F           000F         0000
0001        1001           1001         0001
0002        2002           2002         0002
0003        3003           3003         0003
0004        4004           4004         0004
V2 M09      ACTUAL 8K  CONFIG 8K
```

USER - WRM PROGRAM NAME - SYNT GROUP - CSRD

```
// FOR
*ONE WORD INTEGERS
*LIST ALL
*IOCS(CARD,1403 PRINTER)
C HYDROGENATION OF CODIMER
C PROGRAM TO CALC ERROR AFTER FINDING CONSTANTS
C MECHANISM - NO DISSOCIATION OF HYDROGEN
C
C REAL KH,KU,KS
C DIMENSION PH(20),PU(20),PS(20),REXP(20),RCALC(20),DIFF(20)
C
C ICRD=2
C LPRT=5
C ERROR = 0.0
C PHI=0.0
C
C *** READ CONSTANTS ***
C
C READ(ICRD,100) KH,KU,KS,EK
C
C L=0
C 2 L=L+1
C READ(ICRD,102) REXP(L),PH(L),PU(L),PS(L)
C IF( PH(L) ) 60,30,20
C 20 DENOM = 1.+ KH*PH(L) + KU*PU(L) + KS*PS(L)
C RCALC(L) = EK*KH*KU*PH(L)*PU(L) / DENOM**2
C DIFF(L) = ( REXP(L) - RCALC(L) ) / RCALC(L) * 100.
C PHI = PHI + ( RCALC(L) - REXP(L) )**2
C GO TO 2
C 30 KOUNT = L-1
C WRITE(LPRT,110)
C WRITE(LPRT,111) KH
C WRITE(LPRT,112) KU
C WRITE(LPRT,113) KS
C WRITE(LPRT,114) EK
C WRITE(LPRT,120)
C DO 50 L = 1,KOUNT
C ERROR = ERROR + ABS(DIFF(L))
C 50 WRITE(LPRT,130) L,RCALC(L),REXP(L),PH(L),PU(L),PS(L),DIFF(L)
C XNUM=KOUNT
C ERROR = ERROR/XNUM
C WRITE(LPRT,140) PHI, ERROR
C 60 CALL EXIT
C
C 100 FORMAT( 4F15.0 )
C 102 FORMAT( 10X,4F10.0 )
C 110 FORMAT( 1H1 )
C 111 FORMAT( 6H KH = , F6.4 )
C 112 FORMAT( 6H KU = , F6.4 )
C 113 FORMAT( 6H KS = , F6.4 )
C 114 FORMAT( 6H EK = , F6.4 / )
C 120 FORMAT(3X,50H CALC EXPER PH PU PS /
C 1 3X,20H RXN RATE RXN RATE ,35X,10H PCT ERROR )
C 130 FORMAT(1X,I2,5F10.5,F10.1 )
C 140 FORMAT( // 18H PHI = , F10.6
C 1 / 18H AVG PCT ERROR = , F10.1 )
C
C END
C VARIABLE ALLOCATIONS
C PH(R )=0026-0000 PU(R )=004E-0028 PS(R )=0076-0050 REXP(R )=0
C KH(R )=00F0 KU(R )=00F2 KS(R )=00F4 ERROR(R )=0
C DENOM(R )=00FC XNUM(R )=00FE ICRD(I )=0104 LPRT(I )=0
```

STATEMENT ALLOCATIONS

100	=0114	102	=0117	110	=011B	111	=011E	112	=0124	113	=012A
2	=018D	20	=01DC	30	=0229	50	=0264	60	=0294		

KH = 0.3440
 KU = 0.5450
 KS = 0.4860
 EK = 0.7170

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00300	0.00285	0.48200	0.10000	0.50800	-5.1
2	0.03066	0.03006	2.45900	0.52700	0.51500	-1.9
3	0.03076	0.03072	2.45000	0.53000	0.51500	-0.1
4	0.00445	0.00486	0.47700	0.49400	2.53800	9.1
5	0.01302	0.01393	0.51400	0.54000	0.45500	6.9
6	0.01223	0.01048	0.47300	0.55200	0.47300	-14.3
7	0.01226	0.01453	0.47000	0.55800	0.47300	18.5
8	0.00324	0.00296	0.10400	0.56200	0.44000	-8.7
9	0.02168	0.02177	0.45000	2.84000	0.23000	0.4
10	0.01952	0.01824	0.40900	2.81000	0.28900	-6.5
11	0.01431	0.00921	0.48400	1.07500	0.94200	-35.6
12	0.01791	0.02483	0.35700	1.59000	0.15300	38.6

PHI = 0.000085
 AVG PCT ERROR = 12.1

Synthetic Data with 15% Error - Result of Non-linear Regression
mechanism(d) - 275°C

119.

KH = 0.2060
KU = 0.6400
KS = 0.2160
EK = 0.9910

	CALC	EXPER	PH	PU	PS	PCT ERROR
	RXN RATE	RXN RATE				
1	0.00390	0.00554	0.47800	0.10200	0.52500	42.0
2	0.04436	0.04479	2.50500	0.51800	0.49700	0.9
3	0.04438	0.04398	2.50000	0.51700	0.48500	-0.8
4	0.01794	0.01843	0.42500	2.77000	0.31000	2.7
5	0.01833	0.01722	0.43300	2.80000	0.27000	-6.0
6	0.01658	0.01408	0.48900	0.56200	0.05100	-15.0
7	0.01536	0.00956	0.54600	0.50600	0.44600	-37.7
8	0.01408	0.01593	0.46900	0.55600	0.47500	13.0
9	0.00328	0.00357	0.10000	0.54000	0.46400	8.8
10	0.00671	0.00635	0.42200	0.46200	2.61500	-5.3
11	0.00771	0.00793	0.46700	0.48500	2.55500	2.8
12	0.03289	0.02863	1.49500	0.51100	0.49500	-12.9
13	0.03951	0.04588	1.22200	0.77600	0.10300	16.1

PHI = 0.000106
AVG PCT ERROR = 12.6

Symbolic with 15% error - result of non-linear regression
 mechanism(d) - 325°C

120.

KH = 0.2560
 KU = 0.4920
 KS = 0.0710
 EK = 0.6660

	CALC	EXPER	PH	PU	PS	PCT ERROR
	RXN RATE	RXN RATE				
1	0.01846	0.01810	0.50000	2.73500	0.27000	-1.9
2	0.01149	0.01004	0.48200	0.56000	0.06200	-12.6
3	0.01105	0.00940	0.50100	0.53300	0.46600	-14.8
4	0.01081	0.01273	0.47500	0.55300	0.47100	17.6
5	0.01086	0.01559	0.47600	0.55600	0.47800	43.4
6	0.00263	0.00279	0.10100	0.54800	0.45100	6.0
7	0.02947	0.03450	2.33500	0.55000	0.61000	17.0
8	0.02643	0.02296	2.54000	0.45200	0.51000	-13.1
9	0.02885	0.02784	2.40500	0.52400	0.57200	-3.5
10	0.00274	0.00253	0.48900	0.09800	0.51300	-7.8
11	0.00814	0.01042	0.48000	0.48000	2.55000	27.9
12	0.00704	0.00471	0.55500	0.29900	1.64500	-33.0
13	0.01715	0.01592	0.59900	0.99600	0.90700	-7.1
14	0.01598	0.01339	0.43800	1.52300	0.13600	-16.1
15	0.01713	0.01777	0.47800	1.48000	0.14400	3.6

PHI = 0.000088
 AVG PCT ERROR = 15.0

MECHANISM (h)

EXPERIMENTAL DATA

DISSOCIATION OF H₂ - LINEAR MODEL - 200 DEG C

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RP
RESIDUAL STANDARD DEVIATION	0.2107
STANDARD ERROR OF THE MEAN	0.0608
MULTIPLE R	0.9472
MULTIPLE RSQR	0.8973

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.37015873	0.10667179	0.7751	0.4173
PH ₂	0.95078501	0.17474377	0.8872	0.6370
PO	0.56060064	0.07528787	0.9348	0.9202

STANT 1.6518547

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.12353E 03	0.12353E 03	
REGRESSION	3	0.31045E 01	0.10348E 01	0.23306E 02
ERROR	8	0.35520E 00	0.44400E-01	

$$a = 1.652$$

$$b = 0.951$$

$$c = 0.561$$

$$d = 0.370$$

$$K_H = \left(\frac{b}{a}\right)^2 = \left(\frac{0.951}{1.652}\right)^2 = 0.331$$

$$K_U = \frac{c}{a} = \frac{0.561}{1.652} = 0.339$$

$$K_S = \frac{d}{a} = \frac{0.370}{1.652} = 0.224$$

$$E_k = \frac{1}{a^3 K_H K_U} = 1.977$$

DISSOCIATION OF H₂ - LINEAR MODEL - 275 DEG C

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.2224
STANDARD ERROR OF THE MEAN	0.0416
MULTIPLE R	0.9341
MULTIPLE R SQ	0.8726

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF T	PARTIAL-R	BETA-COEF
PS	0.21892285	0.18135966	0.6677	0.3423
PH ₂	0.64976215	0.17692199	0.7750	0.4646
PH	0.60815811	0.07929322	0.9312	0.9787

CONSTANT	1.7277946
----------	-----------

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.11442E 03	0.11442E 03	
REGRESSION	3	0.30518E 01	0.10172E 01	0.20558E 02
ERROR	9	0.44532E 00	0.49480E-01	

$$a = 1.728$$

$$b = 0.649$$

$$c = 0.608$$

$$d = 0.219$$

$$K_H = \left(\frac{b}{a}\right)^2 = \frac{0.649}{1.728} = 0.141$$

$$K_U = \frac{c}{a} = \frac{0.608}{1.728} = 0.352$$

$$K_S = \frac{d}{a} = \frac{0.219}{1.728} = 0.127$$

$$E_k = \frac{1}{a^3 K_H K_U} = 3.905$$

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.2114
STANDARD ERROR OF THE MEAN	0.0545
MULTIPLE R	0.9110
MULTIPLE RQR	0.8300

VARIABLE ENTERED PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.01406985	0.09286276	0.0456	0.0200
PH ₂	0.59548163	0.15171864	0.7639	0.4986
PH	0.59406566	0.09219306	0.8893	0.8686

KSFANT 2.1657953

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.14899E 03	0.14899E 03	
REGRESSION	3	0.24016E 01	0.80053E 00	0.17910E 02
ERROR	11	0.49165E 00	0.44696E-01	

$$a = 2.166$$

$$b = 0.595$$

$$c = 0.594$$

$$d = 0.014$$

$$K_H = \left(\frac{b}{a}\right)^2 = \left(\frac{0.595}{2.166}\right)^2 = 0.075$$

$$K_V = \frac{c}{a} = \frac{0.594}{2.166} = 0.274$$

$$K_S = \frac{d}{a} = \frac{0.014}{2.166} = 0.006$$

$$E_k = \frac{1}{a^3 K_H K_V} = 4.788$$

Synthetic Experimental Reaction Rate - Results of Linear Regression
 Dissociation of H_2

200°C

KH = 0.3310
 KU = 0.3390
 KS = 0.2240
 EK = 1.9770

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00288	0.00353 ✓	0.48200	0.510000	0.50800	22.2
2	0.02713	0.02500 ✓	2.45900	0.52700	0.51500	-7.8
3	0.02721	0.03200 ✓	2.45000	0.53000	0.51500	17.5
4	0.00538	0.00553 ✓	0.47700	0.49400	2.53800	2.7
5	0.01258	0.00870 ✓	0.51400	0.54000	0.45500	-30.8
6	0.01202	0.01392 ✓	0.47300	0.55200	0.47300	15.7
7	0.01206	0.00960 ✓	0.47000	0.55800	0.47300	-20.4
8	0.00404	0.00514 ✓	0.10400	0.56200	0.44000	27.1
9	0.02050	0.01920 ✓	0.45000	2.84000	0.23000	-6.3
10	0.01878	0.02060 ✓	0.40900	2.81000	0.28900	9.6
11	0.01496	0.01310 ✓	0.48400	1.07500	0.94200	-12.4
12	0.01787	0.01860 ✓	0.35700	1.59000	0.15300	4.0

PHI = 0.000062
 AVG PCT ERROR = 14.7

Experimental Data - Results of Linear Regression
 Dissociation of H₂

275°C

125.

KH = 0.1410
 KU = 0.3520
 KS = 0.1270
 EK = 3.9050

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00373	0.00298	0.47800	0.10200	0.52500	-20.2
2	0.04038	0.03890	2.50500	0.51800	0.49700	-3.6
3	0.04039	0.04500	2.50000	0.51700	0.48500	11.4
4	0.01978	0.02060	0.42500	2.77000	0.31000	4.1
5	0.02016	0.01850	0.43300	2.80000	0.27000	-8.2
6	0.01687	0.01800	0.48900	0.56200	0.05100	6.6
7	0.01548	0.01030	0.54600	0.50600	0.44600	-33.4
8	0.01458	0.01215	0.46900	0.55600	0.47500	-16.7
9	0.00409	0.00705	0.10000	0.54000	0.46400	72.3
10	0.00718	0.00824	0.42200	0.46200	2.61500	14.6
11	0.00816	0.00734	0.46700	0.48500	2.55500	-10.1
12	0.03003	0.03190	1.49500	0.51100	0.49500	6.1
13	0.03732	0.04350	1.22200	0.77600	0.10300	16.5

PHI = 0.000113
 AVG PCT ERROR = 17.2

dissociation of H₂

325°C

126.

KH = 0.0750
 KU = 0.2740
 KS = 0.0060
 EK = 4.7880

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.01829	0.02010	0.50000	2.73500	0.27000	9.8
2	0.01094	0.01140	0.48200	0.56000	0.06200	4.1
3	0.01085	0.01340	0.50100	0.53300	0.46600	23.4
4	0.01066	0.00946	0.47500	0.55300	0.47100	-11.3
5	0.01072	0.00871	0.47600	0.55600	0.47800	-18.7
6	0.00285	0.00250	0.10100	0.54800	0.45100	-12.4
7	0.03247	0.03380	2.33500	0.55000	0.61000	4.0
8	0.02956	0.02860	2.54000	0.45200	0.51000	-3.2
9	0.03193	0.02970	2.40500	0.52400	0.57200	-7.0
10	0.00258	0.00440	0.48900	0.09800	0.51300	70.0
11	0.00949	0.01106	0.48000	0.48000	2.55500	16.4
12	0.00750	0.00533	0.55500	0.29900	1.64500	-28.9
13	0.01773	0.01885	0.59900	0.99600	0.90700	6.2
14	0.01604	0.01414	0.43800	1.52300	0.13600	-11.8
15	0.01713	0.01590	0.47800	1.48000	0.14400	-7.1

PHI = 0.000040
 AVG PCT ERROR = 15.6

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// JOB F 1001 2002 3003 4004 F 2002

FUN

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - LSEST GROUP - CSRD

// FOR

*ONE WORD INTEGERS

*LIST ALL

```

SUBROUTINE FUN(BB)
DIMENSION BB(10)
COMMON KEY,MJM,ND,NF,NFD,NI,NP,PHIZ,SL,B(10),F( 40),G(10),S(10),
1 Y( 40),A(10,10),X(40,16),P(1,10),IPRIN,ILM,MAT,MAR,IPART,
2 FF( 40),KPOIN,NR,NW
DO 1 I=1,ND
DENOM = 1+(BB(1)*X(I,1))**0.5 + BB(2)*X(I,2) + BB(3)*X(I,3)
1 FF(I) =BB(1)*BB(2)* BB(4)*X(I,1)*X(I,2) / DENOM**3
RETURN
END

```

VARIABLE ALLOCATIONS

KEY(IC)=7FFF	MJM(IC)=7FFE	ND(IC)=7FFD	NF(IC)=7FFC
NP(IC)=7FF9	PHIZ(RC)=7FF6	SL(RC)=7FF4	B(RC)=7FF2-7
S(RC)=7F7A-7F68	Y(RC)=7F66-7F18	A(RC)=7F16-7E50	X(RC)=7E4E-7
ILM(IC)=793A	MAT(IC)=7939	MAR(IC)=7938	IPART(IC)=7937
NR(IC)=78E4	NW(IC)=78E3	DENOM(R)=0000	I(I)=0008

STATEMENT ALLOCATIONS

1 =005D

FEATURES SUPPORTED

ONE WORD INTEGERS

CALLED SUBPROGRAMS

FAXB	FADD	FMPYX	FLD	FLDX	FSTO	FSTOX	FDVR	FAXI	FLOA
------	------	-------	-----	------	------	-------	------	------	------

REAL CONSTANTS

.500000E 00=0010

INTEGER CONSTANTS

1=0012 3=0013

CORE REQUIREMENTS FOR FUN

COMMON 1822 VARIABLES 16 PROGRAM 120

RELATIVE ENTRY POINT ADDRESS IS 0014 (HEX)

END OF COMPILATION

// DUP

```

*DELETE          FUN          2002
CART ID 2002    DB ADDR 3DA4    DB CNT  000A

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*STORE          WS   UA   FUN          2002 2002
CART ID 2002    DB ADDR 3E34    DB CNT  000A

```

// JOB F 1001 2002 3003 4004 F 2002

PART

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - LSEST GROUP - CSRD

// FOR
*ONE WORD INTEGERS
*LIST ALL

```

SUBROUTINE PART
COMMON KEY,MJM,ND,NF,NFD,NI,NP,PHIZ,SL,B(10),F( 40),G(10),S(10),
1 Y( 40),A(10,10),X(40,16),P(1,10),IPRIN,ILM,MAT,MAR,IPART,
2 FF( 40),KPOIN,NR,NW
1 K=KPOIN
DENOM = 1. + (B(1)*X(K,1) )**0.5 + B(2)*X(K,2) + B(3)*X(K,3)
P(1,1)= B(2)*B(4)*X(K,1)*X(K,2)*(DENOM-1.5*B(1)**0.5*X(K,1)**0.5)
/ DENOM**4
1 P(1,2)= B(1)*B(4)*X(K,1)*X(K,2)*(DENOM-3.0*B(2)*X(K,2)) /DENOM**4
P(1,3)= 3.0*B(1)*B(2)*B(4)*X(K,1)*X(K,2)*X(K,3) / DENOM**4
P(1,4)= B(1)*B(2)*X(K,1)*X(K,2) / DENOM**3
RETURN
END

```

VARIABLE ALLOCATIONS

KEY(IC)=7FFF	MJM(IC)=7FFE	ND(IC)=7FFD	NF(IC)=7FFC
NP(IC)=7FF9	PHIZ(RC)=7FF6	SL(RC)=7FF4	B(RC)=7FF2-7FE0
S(RC)=7F7A-7F68	Y(RC)=7F66-7F18	A(RC)=7F16-7E50	X(RC)=7E4E-7950
ILM(IC)=793A	MAT(IC)=7939	MAR(IC)=7938	IPART(IC)=7937
NR(IC)=78E4	NW(IC)=78E3	DENOM(R)=0000	K(I)=0008

UNREFERENCED STATEMENTS

1

STATEMENT ALLOCATIONS

1 =0018

FEATURES SUPPORTED
ONE WORD INTEGERS

CALLED SUBPROGRAMS

FAXB	FADD	FMPY	FMPYX	FLD	FLDX	FSTO	FSTOX	FSBR	FOVR
------	------	------	-------	-----	------	------	-------	------	------

REAL CONSTANTS

.100000E 01=0010	.500000E 00=0012	.150000E 01=0014	.300000E 01=0016
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INTEGER CONSTANTS

4=0018	3=0019
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CORE REQUIREMENTS FOR PART

COMMON	1822	VARIABLES	16	PROGRAM	236
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RELATIVE ENTRY POINT ADDRESS IS 001A (HEX)

END OF COMPILATION

// DUP

*DELETE	PART	2002
CART ID 2002	DB ADDR 3DA4	DB CNT 0012

*STORE	WS	UA	PART	2002	2002
CART ID 2002	DB ADDR 3E2C	DB CNT 0012			

EXPERIMENTAL DATA - DISASSOCIATION ...
 Initial Parameters from Linear Regression

DEPENDENT	INDEPENDENT		
	1	2	3
0.35300E-02	0.48200E 00	0.10000E 00	0.50800E 00
0.25000E-01	0.24590E 01	0.52700E 00	0.51500E 00
0.32000E-01	0.24500E 01	0.53000E 00	0.51500E 00
0.55300E-02	0.47700E 00	0.49400E 00	0.25380E 01
0.87000E-02	0.51400E 00	0.54000E 00	0.45500E 00
0.13920E-01	0.47300E 00	0.55200E 00	0.47300E 00
0.96000E-02	0.47000E 00	0.55800E 00	0.47300E 00
0.51400E-02	0.10400E 00	0.56200E 00	0.44000E 00
0.19200E-01	0.45000E 00	0.28400E 01	0.23000E 00
0.20600E-01	0.40900E 00	0.28100E 01	0.28900E 00
0.13100E-01	0.48400E 00	0.10750E 01	0.94200E 00
0.18600E-01	0.35700E 00	0.15900E 01	0.15300E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.162864E-04 PARAMETERS	SQRT(PHI)/ND= 0.66072E-03 0.33100E 00	0.33900E 00	LAMBDA= 0.10000E-01 0.22400E 00	0.19770E 01	MATRIX
PHI= 0.62863E-04 PARAMETERS	SQRT(PHI)/ND= 0.66071E-03 0.33081E 00	0.33928E 00	LAMBDA= 0.10000E 02 0.22311E 00	0.19779E 01	MATRIX
PHI= 0.62495E-04 PARAMETERS	SQRT(PHI)/ND= 0.65878E-03 0.33081E 00	0.33928E 00	LAMBDA= 0.99999E-02 0.23533E 00	0.19821E 01	MATRIX
PHI= 0.60330E-04 PARAMETERS	SQRT(PHI)/ND= 0.64727E-03 0.26427E 00	0.32600E 00	LAMBDA= 0.99999E-02 0.20314E 00	0.23015E 01	MATRIX
PHI= 0.60300E-04 PARAMETERS	SQRT(PHI)/ND= 0.64711E-03 0.26389E 00	0.32509E 00	LAMBDA= 0.99999E 01 0.20061E 00	0.22996E 01	MATRIX
PHI= 0.60295E-04 PARAMETERS	SQRT(PHI)/ND= 0.64708E-03 0.26384E 00	0.32498E 00	LAMBDA= 0.99999E 02 0.20031E 00	0.22993E 01	MATRIX
PHI= 0.60291E-04 PARAMETERS	SQRT(PHI)/ND= 0.64706E-03 0.26379E 00	0.32487E 00	LAMBDA= 0.99999E 02 0.20002E 00	0.22991E 01	MATRIX
PHI= 0.60287E-04 PARAMETERS	SQRT(PHI)/ND= 0.64703E-03 0.26374E 00	0.32477E 00	LAMBDA= 0.99999E 02 0.19973E 00	0.22988E 01	MATRIX
PHI= 0.60283E-04 PARAMETERS	SQRT(PHI)/ND= 0.64702E-03 0.26369E 00	0.32467E 00	LAMBDA= 0.99999E 02 0.19944E 00	0.22986E 01	MATRIX
PHI= 0.60281E-04 PARAMETERS	SQRT(PHI)/ND= 0.64700E-03 0.26364E 00	0.32456E 00	LAMBDA= 0.99999E 02 0.19915E 00	0.22983E 01	MATRIX
PHI= 0.60278E-04 PARAMETERS	SQRT(PHI)/ND= 0.64699E-03 0.26360E 00	0.32446E 00	LAMBDA= 0.99999E 02 0.19886E 00	0.22981E 01	MATRIX
PHI= 0.60276E-04 PARAMETERS	SQRT(PHI)/ND= 0.64698E-03 0.26355E 00	0.32436E 00	LAMBDA= 0.99999E 02 0.19857E 00	0.22978E 01	MATRIX
PHI= 0.60275E-04 PARAMETERS	SQRT(PHI)/ND= 0.64697E-03 0.26350E 00	0.32426E 00	LAMBDA= 0.99999E 02 0.19828E 00	0.22976E 01	MATRIX
PHI= 0.60274E-04 PARAMETERS	SQRT(PHI)/ND= 0.64697E-03 0.26346E 00	0.32416E 00	LAMBDA= 0.99999E 02 0.19800E 00	0.22974E 01	MATRIX
PHI= 0.60273E-04 PARAMETERS	SQRT(PHI)/ND= 0.64696E-03 0.26341E 00	0.32406E 00	LAMBDA= 0.99999E 02 0.19771E 00	0.22971E 01	MATRIX
PHI= 0.60273E-04 PARAMETERS	SQRT(PHI)/ND= 0.64696E-03 0.26337E 00	0.32396E 00	LAMBDA= 0.99999E 02 0.19743E 00	0.22969E 01	MATRIX
PHI= 0.60273E-04 PARAMETERS	SQRT(PHI)/ND= 0.64696E-03 0.26336E 00	0.32395E 00	LAMBDA= 0.99999E 03 0.19740E 00	0.22969E 01	MATRIX
PHI= 0.60273E-04 PARAMETERS	SQRT(PHI)/ND= 0.64696E-03 0.26336E 00	0.32394E 00	LAMBDA= 0.99999E 03 0.19737E 00	0.22969E 01	MATRIX
PHI= 0.60273E-04 PARAMETERS	SQRT(PHI)/ND= 0.64696E-03 0.26335E 00	0.32393E 00	LAMBDA= 0.99999E 03 0.19734E 00	0.22968E 01	MATRIX
PHI= 0.60273E-04 PARAMETERS	SQRT(PHI)/ND= 0.64696E-03 0.26335E 00	0.32392E 00	LAMBDA= 0.99999E 03 0.19731E 00	0.22968E 01	MATRIX

PHI= 0.60273E-04 Sqrt(PHI)/ND= 0.64696E-03 LAMBDA= 0.99999E 02 MATRI
 PARAMETERS 0.26335E 00 0.32392E 00 0.19731E 00 0.22968E 01

PHI= 0.60272E-04 Sqrt(PHI)/ND= 0.64696E-03 LAMBDA= 0.99999E 02 MATRI
 PARAMETERS 0.26335E 00 0.32392E 00 0.19731E 00 0.22968E 01

ALGORITHM CONVERGED

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3
		1		
0.28612E-02	0.66877E-03	0.48200E 00	0.10000E 00	0.50800E 00
0.28336E-01	-0.33360E-02	0.24590E 01	0.52700E 00	0.51500E 00
0.28413E-01	0.35863E-02	0.24500E 01	0.53000E 00	0.51500E 00
0.56412E-02	-0.11129E-03	0.47700E 00	0.49400E 00	0.25380E 01
0.12497E-01	-0.37973E-02	0.51400E 00	0.54000E 00	0.45500E 00
0.11920E-01	0.19996E-02	0.47300E 00	0.55200E 00	0.47300E 00
0.11955E-01	-0.23553E-02	0.47000E 00	0.55800E 00	0.47300E 00
0.38806E-02	0.12593E-02	0.10400E 00	0.56200E 00	0.44000E 00
0.20325E-01	-0.11257E-02	0.45000E 00	0.28400E 01	0.23000E 00
0.18618E-01	0.19815E-02	0.40900E 00	0.28100E 01	0.28900E 00
0.15073E-01	-0.19735E-02	0.48400E 00	0.10750E 01	0.94200E 00
0.17512E-01	0.10870E-02	0.35700E 00	0.15900E 01	0.15300E 00

CORRELATION MATRIX

1.000			
0.589	1.000		
0.796	0.821	1.000	
0.963	0.762	0.853	1.000

21 STEPS

DEPENDENT	INDEPENDENT		
	1	2	3
0.29800E-02	0.47800E 00	0.10200E 00	0.52500E 00
0.38900E-01	0.25050E 01	0.51800E 00	0.49700E 00
0.45000E-01	0.25000E 01	0.51700E 00	0.48500E 00
0.20600E-01	0.42500E 00	0.27700E 01	0.31000E 00
0.18500E-01	0.43300E 00	0.28000E 01	0.27000E 00
0.18000E-01	0.48900E 00	0.56200E 00	0.51000E-01
0.10300E-01	0.54600E 00	0.50600E 00	0.44600E 00
0.12150E-01	0.46900E 00	0.55600E 00	0.47500E 00
0.70500E-02	0.10000E 00	0.54000E 00	0.46400E 00
0.82400E-02	0.42200E 00	0.46200E 00	0.26150E 01
0.73400E-02	0.46700E 00	0.48500E 00	0.25550E 01
0.31900E-01	0.14950E 01	0.51100E 00	0.49500E 00
0.43500E-01	0.12220E 01	0.77600E 00	0.10300E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.11374E-03 PARAMETERS	SQRT(PHI)/ND= 0.82040E-03 0.14100E 00 0.35200E 00	LAMBDA= 0.10000E-01 0.12700E 00 0.39050E 01	MATRIX
PHI= 0.10237E-03 PARAMETERS	SQRT(PHI)/ND= 0.77830E-03 0.14303E 00 0.36034E 00	LAMBDA= 0.10000E 01 0.11946E 00 0.39557E 01	MATRIX
PHI= 0.99339E-04 PARAMETERS	SQRT(PHI)/ND= 0.76668E-03 0.14296E 00 0.36024E 00	LAMBDA= 0.99999E-02 0.14546E 00 0.39577E 01	MATRIX
PHI= 0.97533E-04 PARAMETERS	SQRT(PHI)/ND= 0.75968E-03 0.14375E 00 0.36542E 00	LAMBDA= 0.99999E 00 0.13815E 00 0.39852E 01	MATRIX
PHI= 0.95107E-04 PARAMETERS	SQRT(PHI)/ND= 0.75017E-03 0.14350E 00 0.36545E 00	LAMBDA= 0.99999E-02 0.16056E 00 0.39825E 01	MATRIX
PHI= 0.94317E-04 PARAMETERS	SQRT(PHI)/ND= 0.74705E-03 0.14393E 00 0.36939E 00	LAMBDA= 0.99999E 00 0.15485E 00 0.40026E 01	MATRIX
PHI= 0.92905E-04 PARAMETERS	SQRT(PHI)/ND= 0.74144E-03 0.14372E 00 0.36941E 00	LAMBDA= 0.99999E-02 0.17084E 00 0.40004E 01	MATRIX
PHI= 0.92695E-04 PARAMETERS	SQRT(PHI)/ND= 0.74060E-03 0.14391E 00 0.37240E 00	LAMBDA= 0.99999E 00 0.16600E 00 0.40154E 01	MATRIX
PHI= 0.91721E-04 PARAMETERS	SQRT(PHI)/ND= 0.73670E-03 0.14371E 00 0.37243E 00	LAMBDA= 0.99999E-02 0.17888E 00 0.40132E 01	MATRIX
PHI= 0.91651E-04 PARAMETERS	SQRT(PHI)/ND= 0.73642E-03 0.14379E 00 0.37479E 00	LAMBDA= 0.99999E 00 0.17485E 00 0.40254E 01	MATRIX
PHI= 0.90992E-04 PARAMETERS	SQRT(PHI)/ND= 0.73376E-03 0.14362E 00 0.37481E 00	LAMBDA= 0.99999E-02 0.18521E 00 0.40236E 01	MATRIX
PHI= 0.90975E-04 PARAMETERS	SQRT(PHI)/ND= 0.73370E-03 0.14363E 00 0.37670E 00	LAMBDA= 0.99999E 00 0.18182E 00 0.40339E 01	MATRIX
PHI= 0.90517E-04 PARAMETERS	SQRT(PHI)/ND= 0.73185E-03 0.14349E 00 0.37673E 00	LAMBDA= 0.99999E-02 0.19032E 00 0.40325E 01	MATRIX
PHI= 0.90517E-04 PARAMETERS	SQRT(PHI)/ND= 0.73184E-03 0.14345E 00 0.37824E 00	LAMBDA= 0.99999E 00 0.18745E 00 0.40415E 01	MATRIX
PHI= 0.90193E-04 PARAMETERS	SQRT(PHI)/ND= 0.73054E-03 0.14332E 00 0.37826E 00	LAMBDA= 0.99999E-02 0.19451E 00 0.40403E 01	MATRIX
PHI= 0.90157E-04 PARAMETERS	SQRT(PHI)/ND= 0.73039E-03 0.14334E 00 0.37847E 00	LAMBDA= 0.99999E 01 0.19435E 00 0.40417E 01	MATRIX
PHI= 0.90139E-04 PARAMETERS	SQRT(PHI)/ND= 0.73032E-03 0.14335E 00 0.37864E 00	LAMBDA= 0.99999E 01 0.19412E 00 0.40428E 01	MATRIX
PHI= 0.90132E-04 PARAMETERS	SQRT(PHI)/ND= 0.73029E-03 0.14335E 00 0.37878E 00	LAMBDA= 0.99999E 01 0.19383E 00 0.40436E 01	MATRIX
PHI= 0.90132E-04 PARAMETERS	SQRT(PHI)/ND= 0.73029E-03 0.14335E 00 0.37878E 00	LAMBDA= 0.99999E 03 0.19383E 00 0.40436E 01	MATRIX
PHI= 0.90060E-04	SQRT(PHI)/ND= 0.73000E-03	LAMBDA= 0.99999E-02	MATRIX

PARAMETERS	0.14333E 00	0.37874E 00	0.19665E 00	0.40451E 01	
PHI= 0.89803E-04 PARAMETERS	SQRT(PHI)/ND= 0.72895E-03 0.13000E 00	0.37455E 00	LAMBDA= 0.99999E-02 0.18413E 00	0.43436E 01	MATRI
PHI= 0.89728E-04 PARAMETERS	SQRT(PHI)/ND= 0.72865E-03 0.12985E 00	0.37407E 00	LAMBDA= 0.99999E 01 0.18272E 00	0.43409E 01	MATRI
PHI= 0.89700E-04 PARAMETERS	SQRT(PHI)/ND= 0.72853E-03 0.12973E 00	0.37362E 00	LAMBDA= 0.99999E 01 0.18136E 00	0.43385E 01	MATRI
PHI= 0.89696E-04 PARAMETERS	SQRT(PHI)/ND= 0.72852E-03 0.12971E 00	0.37357E 00	LAMBDA= 0.99999E 02 0.18120E 00	0.43382E 01	MATRI
PHI= 0.89692E-04 PARAMETERS	SQRT(PHI)/ND= 0.72851E-03 0.12970E 00	0.37352E 00	LAMBDA= 0.99999E 02 0.18104E 00	0.43380E 01	MATRI
PHI= 0.89690E-04 PARAMETERS	SQRT(PHI)/ND= 0.72849E-03 0.12968E 00	0.37347E 00	LAMBDA= 0.99999E 02 0.18089E 00	0.43377E 01	MATRI
PHI= 0.89688E-04 PARAMETERS	SQRT(PHI)/ND= 0.72849E-03 0.12967E 00	0.37341E 00	LAMBDA= 0.99999E 02 0.18073E 00	0.43374E 01	MATRI
PHI= 0.89686E-04 PARAMETERS	SQRT(PHI)/ND= 0.72848E-03 0.12965E 00	0.37336E 00	LAMBDA= 0.99999E 02 0.18058E 00	0.43371E 01	MATRI
PHI= 0.89685E-04 PARAMETERS	SQRT(PHI)/ND= 0.72847E-03 0.12964E 00	0.37331E 00	LAMBDA= 0.99999E 02 0.18042E 00	0.43368E 01	MATRI
PHI= 0.89684E-04 PARAMETERS	SQRT(PHI)/ND= 0.72847E-03 0.12962E 00	0.37326E 00	LAMBDA= 0.99999E 02 0.18027E 00	0.43366E 01	MATRI
PHI= 0.89684E-04 PARAMETERS	SQRT(PHI)/ND= 0.72847E-03 0.12961E 00	0.37321E 00	LAMBDA= 0.99999E 02 0.18012E 00	0.43363E 01	MATRI
PHI= 0.89668E-04 PARAMETERS	SQRT(PHI)/ND= 0.72840E-03 0.12958E 00	0.37320E 00	LAMBDA= 0.99999E 01 0.18011E 00	0.43363E 01	MATRI
PHI= 0.89549E-04 PARAMETERS	SQRT(PHI)/ND= 0.72792E-03 0.12936E 00	0.37311E 00	LAMBDA= 0.99999E 00 0.18004E 00	0.43363E 01	MATRI
PHI= 0.89339E-04 PARAMETERS	SQRT(PHI)/ND= 0.72707E-03 0.12871E 00	0.37265E 00	LAMBDA= 0.99999E-01 0.17953E 00	0.43363E 01	MATRI
PHI= 0.89327E-04 PARAMETERS	SQRT(PHI)/ND= 0.72702E-03 0.12849E 00	0.37232E 00	LAMBDA= 0.99999E-01 0.17908E 00	0.43363E 01	MATRI
PHI= 0.89326E-04 PARAMETERS	SQRT(PHI)/ND= 0.72702E-03 0.12846E 00	0.37229E 00	LAMBDA= 0.99999E 00 0.17903E 00	0.43363E 01	MATRI
PHI= 0.89326E-04 PARAMETERS	SQRT(PHI)/ND= 0.72702E-03 0.12846E 00	0.37228E 00	LAMBDA= 0.99999E 01 0.17902E 00	0.43363E 01	MATRI
PHI= 0.89326E-04 PARAMETERS	SQRT(PHI)/ND= 0.72702E-03 0.12845E 00	0.37228E 00	LAMBDA= 0.99999E 00 0.17902E 00	0.43363E 01	MATRI
PHI= 0.89323E-04 PARAMETERS	SQRT(PHI)/ND= 0.72700E-03 0.12840E 00	0.37227E 00	LAMBDA= 0.99999E-01 0.17902E 00	0.43363E 01	MATRI
PHI= 0.89318E-04 PARAMETERS	SQRT(PHI)/ND= 0.72698E-03 0.12832E 00	0.37221E 00	LAMBDA= 0.99999E-02 0.17900E 00	0.43363E 01	MATRI
PHI= 0.89311E-04 PARAMETERS	SQRT(PHI)/ND= 0.72696E-03 0.12845E 00	0.37171E 00	LAMBDA= 0.99999E-03 0.17878E 00	0.43363E 01	MATRI
PHI= 0.89310E-04 PARAMETERS	SQRT(PHI)/ND= 0.72695E-03 0.12854E 00	0.37127E 00	LAMBDA= 0.99999E-03 0.17857E 00	0.43363E 01	MATRI
PHI= 0.89309E-04 PARAMETERS	SQRT(PHI)/ND= 0.72695E-03 0.12851E 00	0.37122E 00	LAMBDA= 0.99999E-02 0.17855E 00	0.43363E 01	MATRI
PHI= 0.89309E-04 PARAMETERS	SQRT(PHI)/ND= 0.72695E-03 0.12850E 00	0.37122E 00	LAMBDA= 0.99999E-01 0.17854E 00	0.43363E 01	MATRI
PHI= 0.89309E-04 PARAMETERS	SQRT(PHI)/ND= 0.72695E-03 0.12850E 00	0.37122E 00	LAMBDA= 0.99999E 00 0.17854E 00	0.43363E 01	MATRI
PHI= 0.89309E-04 PARAMETERS	SQRT(PHI)/ND= 0.72695E-03 0.12850E 00	0.37122E 00	LAMBDA= 0.99999E 00 0.17854E 00	0.43363E 01	MATRI

ALGORITHM CONVERGED

DEPENDENT	DIFFERENCE	INDEPENDENT	1	2	3	4
0.38423E-02	-0.86234E-03	0.47800E 00	0.10200E 00	0.52500E 00	0.49700E 00	
0.42503E-01	-0.36039E-02	0.25050E 01	0.51800E 00	0.48500E 00	0.31000E 00	
0.42549E-01	0.24503E-02	0.25000E 01	0.51700E 00	0.48500E 00	0.27000E 00	
0.19569E-01	0.10301E-02	0.42500E 00	0.27700E 01	0.31000E 00	0.27000E 00	
0.19993E-01	-0.14936E-02	0.43300E 00	0.28000E 01	0.27000E 00	0.51000E-01	
0.17954E-01	0.45049E-04	0.48900E 00	0.56200E 00	0.51000E-01	0.44600E 00	
0.15883E-01	-0.55834E-02	0.54600E 00	0.50600E 00	0.44600E 00	0.47500E 00	
0.14864E-01	-0.27146E-02	0.46900E 00	0.55600E 00	0.47500E 00	0.46400E 00	
0.41001E-02	0.29498E-02	0.10000E 00	0.54000E 00	0.46400E 00	0.26150E 01	
0.61549E-02	0.20851E-02	0.42200E 00	0.46200E 00	0.26150E 01	0.25550E 01	
0.70377E-02	0.30228E-03	0.46700E 00	0.48500E 00	0.25550E 01	0.49500E 00	
0.31253E-01	0.64658E-03	0.14950E 01	0.51100E 00	0.49500E 00	0.10300E 00	
0.39735E-01	0.37649E-02	0.12220E 01	0.77600E 00	0.10300E 00		

CORRELATION MATRIX

1.000			
0.798	1.000		
0.788	0.810	1.000	
0.986	0.872	0.814	1.000

45 STEPS

DEPENDENT	INDEPENDENT		
	1	2	3
0.20100E-01	0.50000E 00	0.27350E 01	0.27000E 00
0.11400E-01	0.48200E 00	0.56000E 00	0.62000E-01
0.13400E-01	0.50100E 00	0.53300E 00	0.46600E 00
0.94600E-02	0.47500E 00	0.55300E 00	0.47100E 00
0.87100E-02	0.47600E 00	0.55600E 00	0.47800E 00
0.25000E-02	0.10100E 00	0.54800E 00	0.45100E 00
0.33800E-01	0.23350E 01	0.55000E 00	0.61000E 00
0.28600E-01	0.25400E 01	0.45200E 00	0.51000E 00
0.29700E-01	0.24050E 01	0.52400E 00	0.57200E 00
0.44000E-02	0.48900E 00	0.98000E-01	0.51300E 00
0.11060E-01	0.48000E 00	0.48000E 00	0.25500E 01
0.53300E-02	0.55500E 00	0.29900E 00	0.16450E 01
0.18850E-01	0.59900E 00	0.99600E 00	0.90700E 00
0.14140E-01	0.43800E 00	0.15230E 01	0.13600E 00
0.15900E-01	0.47800E 00	0.14800E 01	0.14400E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.40106E-04 PARAMETERS	SQRT(PHI)/ND= 0.42219E-03 0.75000E-01	0.27400E 00	LAMBDA= 0.10000E-01 0.60000E-02	0.47880E 01	MATRIX
PHI= 0.39792E-04 PARAMETERS	SQRT(PHI)/ND= 0.42054E-03 0.74788E-01	0.27052E 00	LAMBDA= 0.10000E 01 0.10053E-01	0.47720E 01	MATRIX
PHI= 0.39780E-04 PARAMETERS	SQRT(PHI)/ND= 0.42047E-03 0.74808E-01	0.27057E 00	LAMBDA= 0.99999E-01 0.10062E-01	0.47723E 01	MATRIX
PHI= 0.39769E-04 PARAMETERS	SQRT(PHI)/ND= 0.42041E-03 0.74826E-01	0.27061E 00	LAMBDA= 0.99999E-01 0.10068E-01	0.47725E 01	MATRIX
PHI= 0.39759E-04 PARAMETERS	SQRT(PHI)/ND= 0.42036E-03 0.74843E-01	0.27065E 00	LAMBDA= 0.99999E-01 0.10071E-01	0.47727E 01	MATRIX
PHI= 0.39749E-04 PARAMETERS	SQRT(PHI)/ND= 0.42031E-03 0.74860E-01	0.27069E 00	LAMBDA= 0.99999E-01 0.10072E-01	0.47730E 01	MATRIX
PHI= 0.39741E-04 PARAMETERS	SQRT(PHI)/ND= 0.42027E-03 0.74875E-01	0.27073E 00	LAMBDA= 0.99999E-01 0.10070E-01	0.47732E 01	MATRIX
PHI= 0.39733E-04 PARAMETERS	SQRT(PHI)/ND= 0.42022E-03 0.74890E-01	0.27076E 00	LAMBDA= 0.99999E-01 0.10067E-01	0.47734E 01	MATRIX
PHI= 0.39725E-04 PARAMETERS	SQRT(PHI)/ND= 0.42018E-03 0.74903E-01	0.27080E 00	LAMBDA= 0.99999E-01 0.10061E-01	0.47736E 01	MATRIX
PHI= 0.39718E-04 PARAMETERS	SQRT(PHI)/ND= 0.42015E-03 0.74916E-01	0.27083E 00	LAMBDA= 0.99999E-01 0.10053E-01	0.47738E 01	MATRIX
PHI= 0.39712E-04 PARAMETERS	SQRT(PHI)/ND= 0.42011E-03 0.74927E-01	0.27086E 00	LAMBDA= 0.99999E-01 0.10043E-01	0.47740E 01	MATRIX
PHI= 0.39706E-04 PARAMETERS	SQRT(PHI)/ND= 0.42008E-03 0.74938E-01	0.27089E 00	LAMBDA= 0.99999E-01 0.10031E-01	0.47742E 01	MATRIX
PHI= 0.39700E-04 PARAMETERS	SQRT(PHI)/ND= 0.42005E-03 0.74948E-01	0.27092E 00	LAMBDA= 0.99999E-01 0.10017E-01	0.47744E 01	MATRIX
PHI= 0.39694E-04 PARAMETERS	SQRT(PHI)/ND= 0.42002E-03 0.74958E-01	0.27095E 00	LAMBDA= 0.99999E-01 0.10001E-01	0.47746E 01	MATRIX
PHI= 0.39689E-04 PARAMETERS	SQRT(PHI)/ND= 0.41999E-03 0.74967E-01	0.27097E 00	LAMBDA= 0.99999E-01 0.99841E-02	0.47748E 01	MATRIX
PHI= 0.39684E-04 PARAMETERS	SQRT(PHI)/ND= 0.41997E-03 0.74975E-01	0.27100E 00	LAMBDA= 0.99999E-01 0.99651E-02	0.47750E 01	MATRIX
PHI= 0.39679E-04 PARAMETERS	SQRT(PHI)/ND= 0.41994E-03 0.74982E-01	0.27102E 00	LAMBDA= 0.99999E-01 0.99444E-02	0.47752E 01	MATRIX
PHI= 0.39674E-04 PARAMETERS	SQRT(PHI)/ND= 0.41992E-03 0.74988E-01	0.27104E 00	LAMBDA= 0.99999E-01 0.99222E-02	0.47754E 01	MATRIX
PHI= 0.39670E-04 PARAMETERS	SQRT(PHI)/ND= 0.41989E-03 0.74995E-01	0.27106E 00	LAMBDA= 0.99999E-01 0.98985E-02	0.47756E 01	MATRIX

PHI= 0.39665E-04 PARAMETERS	SQRT(PHI)/ND= 0.41987E-03 0.75000E-01 0.27108E 00	LAMBDA= 0.99999E-01 0.98734E-02 0.47758E 01	MATRIX
PHI= 0.39661E-04 PARAMETERS	SQRT(PHI)/ND= 0.41985E-03 0.75001E-01 0.27108E 00	LAMBDA= 0.99999E-02 0.98734E-02 0.47868E 01	MATRIX
PHI= 0.39656E-04 PARAMETERS	SQRT(PHI)/ND= 0.41982E-03 0.74998E-01 0.27109E 00	LAMBDA= 0.99999E-01 0.98279E-02 0.47869E 01	MATRIX
PHI= 0.39650E-04 PARAMETERS	SQRT(PHI)/ND= 0.41979E-03 0.74994E-01 0.27109E 00	LAMBDA= 0.99999E-01 0.97818E-02 0.47871E 01	MATRIX
PHI= 0.39644E-04 PARAMETERS	SQRT(PHI)/ND= 0.41976E-03 0.74991E-01 0.27109E 00	LAMBDA= 0.99999E-01 0.97352E-02 0.47872E 01	MATRIX
PHI= 0.39639E-04 PARAMETERS	SQRT(PHI)/ND= 0.41973E-03 0.74986E-01 0.27109E 00	LAMBDA= 0.99999E-01 0.96881E-02 0.47874E 01	MATRIX
PHI= 0.39633E-04 PARAMETERS	SQRT(PHI)/ND= 0.41969E-03 0.74982E-01 0.27109E 00	LAMBDA= 0.99999E-01 0.96406E-02 0.47875E 01	MATRIX
PHI= 0.39627E-04 PARAMETERS	SQRT(PHI)/ND= 0.41966E-03 0.74978E-01 0.27110E 00	LAMBDA= 0.99999E-01 0.95925E-02 0.47877E 01	MATRIX

ALGORITHM TERMINATED

PHI= 0.39627E-04 PARAMETERS	SQRT(PHI)/ND= 0.41966E-03 0.74978E-01 0.27110E 00	LAMBDA= 0.99999E 04 0.95925E-02 0.47877E 01	MATRIX
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DEPENDENT	DIFFERENCE	INDEPENDENT	2	3	4
		1			
0.18292E-01	0.18070E-02	0.50000E 00	0.27350E 01	0.27000E 00	
0.10856E-01	0.54384E-03	0.48200E 00	0.56000E 00	0.62000E-01	
0.10733E-01	0.26663E-02	0.50100E 00	0.53300E 00	0.46600E 00	
0.10549E-01	-0.10896E-02	0.47500E 00	0.55300E 00	0.47100E 00	
0.10603E-01	-0.18936E-02	0.47600E 00	0.55600E 00	0.47800E 00	
0.28257E-02	-0.32571E-03	0.10100E 00	0.54800E 00	0.45100E 00	
0.32088E-01	0.17113E-02	0.23350E 01	0.55000E 00	0.61000E 00	
0.29214E-01	-0.61476E-03	0.25400E 01	0.45200E 00	0.51000E 00	
0.31559E-01	-0.18596E-02	0.24050E 01	0.52400E 00	0.57200E 00	
0.25496E-02	0.18503E-02	0.48900E 00	0.98000E-01	0.51300E 00	
0.92298E-02	0.18301E-02	0.48000E 00	0.48000E 00	0.25500E 01	
0.73366E-02	-0.20066E-02	0.55500E 00	0.29900E 00	0.16450E 01	
0.17529E-01	0.13206E-02	0.59900E 00	0.99600E 00	0.90700E 00	
0.15986E-01	-0.18465E-02	0.43800E 00	0.15230E 01	0.13600E 00	
0.17065E-01	-0.11655E-02	0.47800E 00	0.14800E 01	0.14400E 00	

CORRELATION MATRIX

1.000			
0.850	1.000		
0.784	0.820	1.000	
0.987	0.912	0.802	1.000

27 STEPS

// JOB F 1001 2002 3003 4004 F 2002

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - SYNT GROUP - CSRD

```

// FOR
*ONE WORD INTEGERS
*LIST ALL
*IOCS(CARD,1403 PRINTER)
C HYDROGENATION OF CODIMER
C PROGRAM TO CALC ERROR AFTER FINDING CONSTANTS
C MECHANISM - DISSOCIATION OF HYDROGEN
C
REAL KH,KU,KS
C DIMENSION PH(20),PU(20),PS(20),REXP(20),RCALC(20),DIFF(20)
C
ICRD=2
LPRT=5
PHI=0.0
ERROR = 0.0
C
C *** READ CONSTANTS ***
C
READ(ICRD,100) KH,KU,KS,EK
C
L=0
2 L=L+1
READ(ICRD,102) REXP(L),PH(L),PU(L),PS(L)
IF( PH(L) ) 60,30,20
20 DENOM = 1 + (KH*PH(L))*0.5 + KU*PU(L) + KS*PS(L)
RCALC(L) = EK*KH*KU*PH(L)*PU(L) / DENOM**3
DIFF(L) = ( REXP(L) - RCALC(L) ) / RCALC(L) * 100.
PHI = PHI + ( RCALC(L) - REXP(L) )**2
GO TO 2
30 KOUNT = L-1
WRITE(LPRT,110)
WRITE(LPRT,111) KH
WRITE(LPRT,112) KU
WRITE(LPRT,113) KS
WRITE(LPRT,114) EK
WRITE(LPRT,120)
DO 50 L = 1,KOUNT
ERROR = ERROR + ABS(DIFF(L))
50 WRITE(LPRT,130) L,RCALC(L),REXP(L),PH(L),PU(L),PS(L),DIFF(L)
XNUM=KOUNT
ERROR = ERROR / XNUM
WRITE(LPRT,140) PHI, ERROR
60 CALL EXIT
C
100 FORMAT( 4F15.0 )
110 FORMAT( 1H1 )
102 FORMAT( 10X,4F10.0 )
111 FORMAT( 6H KH = , F6.4 )
112 FORMAT( 6H KU = , F6.4 )
113 FORMAT( 6H KS = , F6.4 )
114 FORMAT( 6H EK = , F6.4 / )
120 FORMAT(3X,50H CALC EXPER PH PU PS
1 3X,20H RXN RATE RXN RATE ,35X,10H PCT ERROR )
130 FORMAT(1X,I2,5F10.5,F10.1 )
140 FORMAT( // 18H PHI = , F10.6
1 / 18H AVG PCT ERROR = , F10.1 )
END
VARIABLE ALLOCATIONS
PH(R )=0026-0000 PU(R )=004E-0028 PS(R )=0076-0050 REXP(R )=
KH(R )=00FO KU(R )=00F2 KS(R )=00F4 PHI(R )=
DENOM(R )=00FC XNUM(R )=00FE ICRD(I )=0106 LPRT(I )=
STATEMENT ALLOCATIONS
100 =0117 110 =011A 102 =011D 111 =0121 112 =0127 113 =012F
2 =01C0 20 =01DF 30 =0234 50 =026F 60 =029F

```

Experimental Data - Results of Non-Linear Regression
 Dissociation of H_2 - 200°C

KH = 0.2630
 KU = 0.3240
 KS = 0.1970
 EK = 2.2970

	CALC	EXPER	PH	PU	PS	PCT ERROR	
	RXN RATE	RXN RATE					
1	0.00286	0.00353	0.48200	0.10000	0.50800	23.4	87
2	0.02833	0.02500	2.45900	0.52700	0.51500	-11.7	-332
3	0.02841	0.03200	2.45000	0.53000	0.51500	12.6	359
4	0.00564	0.00553	0.47700	0.49400	2.53800	-2.0	-11
5	0.01249	0.00870	0.51400	0.54000	0.45500	-30.3	-379
6	0.01191	0.01392	0.47300	0.55200	0.47300	16.8	201
7	0.01195	0.00960	0.47000	0.55800	0.47300	-19.6	-235
8	0.00387	0.00514	0.10400	0.56200	0.44000	32.5	127
9	0.02030	0.01920	0.45000	2.84000	0.23000	-5.4	-110
10	0.01860	0.02060	0.40900	2.81000	0.28900	10.7	200
11	0.01506	0.01310	0.48400	1.07500	0.94200	-13.0	-196
12	0.01749	0.01860	0.35700	1.59000	0.15300	6.2	111

PHI = 0.000060
 AVG PCT ERROR = 15.3

Check Calculation

$$\begin{aligned}
 r_2 &= \frac{EK K_H K_U P_H P_U}{(1 + \sqrt{K_H P_H} + K_U P_U + K_S P_S)^3} \\
 &= \frac{(2.297)(0.263)(0.324)(2.459)(0.527)}{(1 + \sqrt{(0.263)(2.459)} + (0.324)(0.527) + (0.197)(0.515))^3} \\
 &= \frac{0.2536}{(1 + 0.8042 + 0.1707 + 0.1014)^3} = \frac{0.2536}{(2.0763)^3} = 0.02833 \quad \checkmark \text{ OK}
 \end{aligned}$$

Experimental Data - Results of Non-linear Regression
 Dissociation of H_2 - 275°C

KH = 0.1280
 KU = 0.3710
 KS = 0.1780
 EK = 4.3360

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR	
1	0.00383	0.00298	0.47800	0.10200	0.52500	-22.2	-85
2	0.04241	0.03890	2.50500	0.51800	0.49700	-8.2	-351
3	0.04245	0.04500	2.50000	0.51700	0.48500	5.9	255
4	0.01951	0.02060	0.42500	2.77000	0.31000	5.5	109
5	0.01993	0.01850	0.43300	2.80000	0.27000	-7.1	-143
6	0.01789	0.01800	0.48900	0.56200	0.05100	0.5	11
7	0.01583	0.01030	0.54600	0.50600	0.44600	-34.9	-553
8	0.01482	0.01215	0.46900	0.55600	0.47500	-18.0	-267
9	0.00408	0.00705	0.10000	0.54000	0.46400	72.5	297
10	0.00614	0.00824	0.42200	0.46200	2.61500	34.0	210
11	0.00702	0.00734	0.46700	0.48500	2.55500	4.4	32
12	0.03117	0.03190	1.49500	0.51100	0.49500	2.3	73
13	0.03962	0.04350	1.22200	0.77600	0.10300	9.7	388

PHI = 0.000089
 AVG PCT ERROR = 17.3

MECHANISM (h)

SYNTHETIC DATA

DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.0008
STANDARD ERROR OF THE MEAN	0.0002
MULTIPLE R	0.9999
MULTIPLE RSQR	0.9999

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.72338628	0.00042313	0.9999	0.4785
PH2	1.26176739	0.00069316	0.9999	0.4959
PU	1.08796882	0.00029864	0.9999	1.0477

CONSTANT 1.9715628

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN REGRESSION	1	0.24648E 03	0.24648E 03	
REGRESSION	3	0.10052E 02	0.33508E 01	0.47961E 0
ERROR	8	0.55891E-05	0.69864E-06	

$a = 1.9716$

$$k_H = \left(\frac{b}{a}\right)^2 = \left(\frac{1.2618}{1.9716}\right)^2 = 0.4096 \quad \text{vs } 0.4100$$

$b = 1.2618$

$$k_U = \frac{c}{a} = \frac{1.0880}{1.9716} = 0.5518 \quad \text{vs } 0.5520$$

$c = 1.0880$

$$k_S = \frac{d}{a} = \frac{0.7234}{1.9716} = 0.3669 \quad \text{vs } 0.3670$$

$d = 0.7234$

$$E_R = \frac{1}{a^3 k_H k_U} = 0.5773 \quad \text{vs } 0.5770$$

Synthetic Reaction Rates = ~~RT~~ with no error -
 mechanism (h) - 275°C

DISSOCIATION OF HYDROGEN LINEAR REGRESSION

141.

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.0022
STANDARD ERROR OF THE MEAN	0.0006
MULTIPLE R	0.9999
MULTIPLE RSQR	0.9999

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.37678605	0.00080918	0.9999	0.3383
PH2	0.99135852	0.00175067	0.9999	0.4071
PU	1.15206933	0.00078863	0.9999	1.0647
CONSTANT	1.9830765			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN REGRESSION	1	0.21806E 03	0.21806E 03	0.72212E 0
REGRESSION	3	0.10603E 02	0.35344E 01	
ERROR	9	0.44051E-04	0.48945E-05	

$$a = 1.98307$$

$$K_H = \left(\frac{b}{a}\right)^2 = \left(\frac{0.99136}{1.98307}\right)^2 = 0.2499 \quad \text{vs. } 0.2500$$

$$b = 0.99136$$

$$K_U = \frac{c}{a} = \frac{1.15207}{1.98307} = 0.5809 \quad \text{vs. } 0.5810$$

$$c = 1.15207$$

$$K_S = \frac{d}{a} = \frac{0.37679}{1.98307} = 0.1900 \quad \text{vs. } 0.1900$$

$$d = 0.37679$$

$$E_R = \frac{1}{a^3 K_H K_U} = 0.9833 \quad \text{vs. } 0.9830$$

mechanism(h) - 375°C
 DISSOCIATION OF HYDROGEN LINEAR REGRESSION

142.

REGRESSION ANALYSIS

DEPENDENT VARIABLE RR
 RESIDUAL STANDARD DEVIATION 0.0026
 STANDARD ERROR OF THE MEAN 0.0006
 MULTIPLE R 0.9999
 MULTIPLE RSQR 0.9999

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.04265237	0.00114869	0.9960	0.0371
PH2	1.06947136	0.00187348	0.9999	0.5482
PU	1.07065367	0.00113744	0.9999	0.9583
CONSTANT	2.3749313			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN REGRESSION	1	0.25955E 03	0.25955E 03	0.37754E 01
REGRESSION	3	0.77196E 01	0.25732E 01	
ERROR	11	0.74971E-04	0.68155E-05	

$a = 2.37493$
 $b = 1.06947$
 $c = 1.07065$
 $d = 0.04265$

$K_H = \left(\frac{b}{a}\right)^2 = \left(\frac{1.06947}{2.37493}\right)^2 = 0.2028 \quad \text{vs. } .2030$
 $K_U = \frac{c}{a} = \frac{1.07065}{2.37493} = 0.4508 \quad \text{vs. } .4510$
 $K_S = \frac{d}{a} = \frac{0.04265}{2.37493} = 0.0179 \quad \text{vs. } .018$
 $E_k = \frac{1}{a^3 K_H K_U} = 0.8166 \quad \text{vs. } .8160$

```
// JOB          F 1001 2002 3003 4004      F 2002
LOG DRIVE      CART SPEC      CART AVAIL  PHY DRIVE
 0000          000F           000F         0000
 0001          1001           1001         0001
 0002          2002           2002         0002
 0003          3003           3003         0003
 0004          4004           4004         0004
```

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - SYNT GROUP - CSRD

```
// FOR
*ONE WORD INTEGERS
*LIST ALL
*IOCS(CARD,1403 PRINTER)
C HYDROGENATION OF CODIMER
C PROGRAM TO CALC ERROR AFTER FINDING CONSTANTS
C MECHANISM - DISSOCIATION OF HYDROGEN
C
C REAL KH,KU,KS
C DIMENSION PH(20),PU(20),PS(20),REXP(20),RCALC(20),DIFF(20)
C
C ICRD=2
C LPRT=5
C PHI=0.0
C ERROR = 0.0
C
C *** READ CONSTANTS ***
C
C READ(ICRD,100) KH,KU,KS,EK
C
C L=0
C 2 L=L+1
C READ(ICRD,102) REXP(L),PH(L),PU(L),PS(L)
C IF( PH(L) ) 60,30,20
C 20 DENOM = 1 + (KH*PH(L))*0.5 + KU*PU(L) + KS*PS(L)
C RCALC(L) = EK*KH*KU*PH(L)*PU(L) / DENOM**3
C DIFF(L) = ( REXP(L) - RCALC(L) ) / RCALC(L) * 100.
C PHI = PHI + ( RCALC(L) - REXP(L) )**2
C GO TO 2
C 30 KOUNT = L-1
C WRITE(LPRT,110)
C WRITE(LPRT,111) KH
C WRITE(LPRT,112) KU
C WRITE(LPRT,113) KS
C WRITE(LPRT,114) EK
C WRITE(LPRT,120)
C DO 50 L = 1, KOUNT
C ERROR = ERROR + ABS(DIFF(L))
C 50 WRITE(LPRT,130) L,RCALC(L),REXP(L),PH(L),PU(L),PS(L),DIFF(L)
C XNUM=KOUNT
C ERROR = ERROR / XNUM
C WRITE(LPRT,140) PHI, ERROR
C 60 CALL EXIT
C
C 100 FORMAT( 4F15.0 )
C 110 FORMAT( 1H1 )
C 102 FORMAT( 10X,4F10.0 )
C 111 FORMAT( 6H KH = , F6.4 )
C 112 FORMAT( 6H KU = , F6.4 )
C 113 FORMAT( 6H KS = , F6.4 )
C 114 FORMAT( 6H EK = , F6.4 / )
C 120 FORMAT( 3X,50H CALC EXPR PH PU PS
C 1 3X,20H RXN RATE RXN RATE ,35X,10H PCT ERROR )
C 130 FORMAT( 1X,12,5F10.5,F10.1 )
C 140 FORMAT( // 18H PHI = , F10.6
C 1 / 18H AVG PCT ERROR = , F10.1 )
C
C END
C VARIABLE ALLOCATIONS
C PH(R )=0026-0000 PU(R )=004E-0028 PS(R )=0076-0050 REXP(R )
C KH(R )=00F0 KU(R )=00F2 KS(R )=00F4 PHI(R )
C DENOM(R )=00FC XNUM(R )=00FE ICRD(I )=0106 LPRT(I )
C
C STATEMENT ALLOCATIONS
C 100 =0117 110 =011A 102 =011D 111 =0121 112 =0127 113 =012
C 2 =01C0 20 =01DF 30 =0234 50 =026F 60 =029F
```

Disassociation of H_2
200°C

Check Error in Data 144.
Should be 157.

KH = 0.4100
KU = 0.5520
KS = 0.3670
EK = 0.5770

	CALC	EXPER	PH	PU	PS	PCT ERROR
	RXN RATE	RXN RATE				
1	0.00131	0.00123	0.48200	0.10000	0.50800	-6.0
2	0.01104	0.01214	2.45900	0.52700	0.51500	9.9
3	0.01106	0.01239	2.45000	0.53000	0.51500	11.9
4	0.00166	0.00151	0.47700	0.49400	2.53800	-9.0
5	0.00508	0.00549	0.51400	0.54000	0.45500	7.9
6	0.00482	0.00561	0.47300	0.55200	0.47300	16.2
7	0.00483	0.00575	0.47000	0.55800	0.47300	18.9
8	0.00161	0.00143	0.10400	0.56200	0.44000	-11.0
9	0.00570	0.00598	0.45000	2.84000	0.23000	4.9
10	0.00520	0.00504	0.40900	2.81000	0.28900	-3.0
11	0.00501	0.00310	0.48400	1.07500	0.94200	-38.0
12	0.00596	0.00864	0.35700	1.59000	0.15300	44.9

PHI = 0.000015
AVG PCT ERROR = 15.2

Dissociation of H₂

275°C

Check Error in Data
Should be 15?

145.

KH = 0.2500
KU = 0.5810
KS = 0.1900
EK = 0.8830

	CALC	EXPER	PH	PU	PS	PCT ERROR
	RXN RATE	RXN RATE				
1	0.00183	0.00266	0.47800	0.10200	0.52500	44.9
2	0.01591	0.01750	2.50500	0.51800	0.49700	9.9
3	0.01593	0.01720	2.50000	0.51700	0.48500	7.9
4	0.00562	0.00528	0.42500	2.77000	0.31000	-6.0
5	0.00571	0.00491	0.43300	2.80000	0.27000	-14.0
6	0.00735	0.00625	0.48900	0.56200	0.05100	-15.0
7	0.00663	0.00411	0.54600	0.50600	0.44600	-37.9
8	0.00617	0.00692	0.46900	0.55600	0.47500	11.9
9	0.00182	0.00191	0.10000	0.54000	0.46400	4.9
10	0.00273	0.00243	0.42200	0.46200	2.61500	-11.0
11	0.00309	0.00300	0.46700	0.48500	2.55500	-3.0
12	0.01220	0.01110	1.49500	0.51100	0.49500	-9.0
13	0.01468	0.01747	1.22200	0.77600	0.10300	18.9

PHI = 0.000022
AVG PCT ERROR = 14.9

Dissociation of H₂

325°C

Check Error in Data
Should be 15% 146.

KH = 0.2030
KU = 0.4510
KS = 0.0180
EK = 0.8160

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00611	0.00592	0.50000	2.73500	0.27000	-3.0
2	0.00524	0.00477	0.48200	0.56000	0.06200	-9.0
3	0.00517	0.00445	0.50100	0.53300	0.46600	-14.0
4	0.00508	0.00605	0.47500	0.55300	0.47100	18.9
5	0.00510	0.00740	0.47600	0.55600	0.47800	44.9
6	0.00151	0.00166	0.10100	0.54800	0.45100	9.9
7	0.01298	0.01402	2.33500	0.55000	0.61000	7.9
8	0.01191	0.00952	2.54000	0.45200	0.51000	-20.0
9	0.01278	0.01138	2.40500	0.52400	0.57200	-11.0
10	0.00139	0.00131	0.48900	0.09800	0.51300	-6.0
11	0.00440	0.00493	0.48000	0.48000	2.55000	11.9
12	0.00367	0.00227	0.55500	0.29900	1.64500	-37.9
13	0.00746	0.00671	0.59900	0.99600	0.90700	-9.9
14	0.00634	0.00539	0.43800	1.52300	0.13600	-15.0
15	0.00679	0.00713	0.47800	1.48000	0.14400	5.0

PHL = 0.000019
AVG PCT ERROR = 15.0

DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.3368
STANDARD ERROR OF THE MEAN	0.0972
MULTIPLE R	0.9599
MULTIPLE RSQR	0.9214

VARIABLE ENTERED PH2

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.94070506	0.17051392	0.8898	0.5803
PH2	1.10871100	0.27932643	0.8143	0.4064
PU	1.10598183	0.12034703	0.9557	0.9933
CONSTANT	1.9204466			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.24452E 03	0.24452E 03	
REGRESSION	3	0.10648E 02	0.35495E 01	0.31286E 0
ERROR	8	0.90761E 00	0.11345E 00	

$$1.9204 \quad K_H = \left(\frac{b}{a}\right)^2 = 0.333$$

$$1.1087 \quad K_U = \frac{F}{a} = 0.576$$

$$1.1060 \quad K_S = \frac{d}{a} = 0.490$$

$$0.9407 \quad E_k = \frac{1}{a^2 k_U k_V} = 0.736$$

DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE RR
 RESIDUAL STANDARD DEVIATION 0.2626
 STANDARD ERROR OF THE MEAN 0.0728
 MULTIPLE R 0.9755
 MULTIPLE RSQR 0.9517

VARIABLE ENTERED

PH2

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.41335660	0.09607550	0.8202	0.3369
PH2	0.87484204	0.20785975	0.8143	0.3261
PU	1.24579882	0.09363527	0.9755	1.0452

CONSTANT 2.0203533

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.22261E 03	0.22261E 03	
REGRESSION	3	0.12244E 02	0.40816E 01	0.59154E
ERROR	9	0.62099E 00	0.68999E-01	

a = 2.0203
 b = 0.8748
 c = 1.2458
 d = 0.4133

$$K_H = \left(\frac{b}{a}\right)^2 = \left(\frac{0.8748}{2.0203}\right)^2 = 0.187$$

$$K_U = \frac{c}{a} = \frac{1.2458}{2.0203} = 0.617$$

$$K_S = \frac{d}{a} = \frac{0.4133}{2.0203} = 0.205$$

$$E_R = \frac{1}{a^3 K_H K_U} = 1.0510$$

DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.2783
STANDARD ERROR OF THE MEAN	0.0718
MULTIPLE R	0.9525
MULTIPLE RSQR	0.9073

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.09158006	0.12248349	0.2199	0.0730
PH2	1.23416924	0.19976601	0.8810	0.5793
PU	1.09502458	0.12128412	0.9386	0.8976
CONSTANT	2.2457914			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.26734E 03	0.26734E 03	
REGRESSION	3	0.83524E 01	0.27841E 01	0.35929E
ERROR	11	0.85239E 00	0.77490E-01	

$a = 2.2458$

$K_H = \left(\frac{b}{a}\right)^2 = 0.302$

$b = 1.2342$

$K_U = \frac{c}{a} = 0.488$

$c = 1.0950$

$K_S = \frac{d}{a} = 0.041$

$d = 0.0916$

$E_R = \frac{1}{a^3 K_H K_U} = 0.599$

// JOB F 1001 2002 3003 4004 F 2002

150.

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - SYNT GROUP - CSRD

// FOR

*ONE WORD INTEGERS

*LIST ALL

*IOCS(CARD,1403 PRINTER)

C HYDROGENATION OF CODIMER
 C PROGRAM TO CALC ERROR AFTER FINDING CONSTANTS
 C MECHANISM - DISSOCIATION OF HYDROGEN
 C

REAL KH,KU,KS
 DIMENSION PH(20),PU(20),PS(20),REXP(20),RCALC(20),DIFF(20)

C ICRD=2
 LPRT=5
 PHI=0.0
 ERROR = 0.0

C *** READ CONSTANTS ***

C READ(ICRD,100) KH,KU,KS,EK

C L=0

2 L=L+1
 READ(ICRD,102) REXP(L),PH(L),PU(L),PS(L)
 IF(PH(L)) 60,30,20
 20 DENOM = 1 + (KH*PH(L))**0.5 + KU*PU(L) + KS*PS(L)
 RCALC(L) = EK*KH*KU*PH(L)*PU(L) / DENOM**3
 DIFF(L) = (REXP(L) - RCALC(L)) / RCALC(L) * 100.
 PHI = PHI + (RCALC(L) - REXP(L))**2

30 KOUNT = L-1
 WRITE(LPRT,110)
 WRITE(LPRT,111) KH
 WRITE(LPRT,112) KU
 WRITE(LPRT,113) KS
 WRITE(LPRT,114) EK
 WRITE(LPRT,120)
 DO 50 L = 1, KOUNT
 ERROR = ERROR + ABS(DIFF(L))
 50 WRITE(LPRT,130) L,RCALC(L),REXP(L),PH(L),PU(L),PS(L),DIFF(L)
 XNUM=KOUNT
 ERROR = ERROR / XNUM
 WRITE(LPRT,140) PHI, ERROR
 60 CALL EXIT

C 100 FORMAT(4F15.0)
 110 FORMAT(1H1)
 102 FORMAT(10X,4F10.0)
 111 FORMAT(6H KH = , F6.4)
 112 FORMAT(6H KU = , F6.4)
 113 FORMAT(6H KS = , F6.4)
 114 FORMAT(6H EK = , F6.4 /)
 120 FORMAT(3X,50H CALC EXPER PH PU PS /
 1 3X,20H RXN RATE RXN RATE ,35X,10H PCT ERROR)
 130 FORMAT(1X,12,5F10.5,F10.1)
 140 FORMAT(// 18H PHI = , F10.6
 1 / 18H AVG PCT ERROR = , F10.1)

END

VARIABLE ALLOCATIONS
 PH(R)=0026-0000 PU(R)=004E-0028 PS(R)=0076-0050 REXP(R)=
 KH(R)=00F0 KU(R)=00F2 KS(R)=00F4 PHI(R)=
 DENOM(R)=00FC XNUM(R)=00FE ICRD(I)=0106 LPRT(I)=

STATEMENT ALLOCATIONS

100	=0117	110	=011A	102	=011D	111	=0121	112	=0127	113	=012C
2	=01C0	20	=01DF	30	=0234	50	=026F	60	=029F		

Mechanism (h) - 200°C

151.

KH = 0.3330
KU = 0.5760
KS = 0.4900
EK = 0.7360

	CALC	EXPER	PH	PU	PS	PCT ERROR
	RXN RATE	RXN RATE				
1	0.00136	0.00123	0.48200	0.10000	0.50800	-9.8
2	0.01227	0.01214	2.45900	0.52700	0.51500	-1.0
3	0.01230	0.01239	2.45000	0.53000	0.51500	0.7
4	0.00132	0.00151	0.47700	0.49400	2.53800	13.7
5	0.00530	0.00549	0.51400	0.54000	0.45500	3.6
6	0.00499	0.00561	0.47300	0.55200	0.47300	12.3
7	0.00500	0.00575	0.47000	0.55800	0.47300	14.9
8	0.00160	0.00143	0.10400	0.56200	0.44000	-10.6
9	0.00585	0.00598	0.45000	2.84000	0.23000	2.3
10	0.00529	0.00504	0.40900	2.81000	0.28900	-4.6
11	0.00480	0.00310	0.48400	1.07500	0.94200	-35.3
12	0.00628	0.00864	0.35700	1.59000	0.15300	37.4

PHI = 0.000009
AVG PCT ERROR = 12.2

mechanism (h) - ~~275~~ 275° C

152.

KH = 0.1870
KU = 0.6170
KS = 0.2050
EK = 1.0510

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00186	0.00266	0.47800	0.10200	0.52500	42.8
2	0.01684	0.01750	2.50500	0.51800	0.49700	3.9
3	0.01687	0.01720	2.50000	0.51700	0.48500	1.9
4	0.00500	0.00528	0.42500	2.77000	0.31000	5.5
5	0.00509	0.00491	0.43300	2.80000	0.27000	-3.4
6	0.00729	0.00625	0.48900	0.56200	0.05100	-14.2
7	0.00654	0.00411	0.54600	0.50600	0.44600	-37.1
8	0.00603	0.00692	0.46900	0.55600	0.47500	14.6
9	0.00170	0.00191	0.10000	0.54000	0.46400	12.1
10	0.00254	0.00243	0.42200	0.46200	2.61500	-4.2
11	0.00288	0.00300	0.46700	0.48500	2.55500	3.9
12	0.01258	0.01110	1.49500	0.51100	0.49500	-11.7
13	0.01486	0.01747	1.22200	0.77600	0.10300	17.6

PHI = 0.000018
AVG PCT ERROR = 13.3

Association of the mechanism (h)

KH = 0.3020
 KU = 0.4880
 KS = 0.0410
 EK = 0.5990

325°C

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00590	0.00592	0.50000	2.73500	0.27000	0.3
2	0.00523	0.00477	0.48200	0.56000	0.06200	-8.8
3	0.00507	0.00445	0.50100	0.53300	0.46600	-12.3
4	0.00499	0.00605	0.47500	0.55300	0.47100	21.1
5	0.00501	0.00740	0.47600	0.55600	0.47800	47.6
6	0.00156	0.00166	0.10100	0.54800	0.45100	5.9
7	0.01167	0.01402	2.33500	0.55000	0.61000	20.0
8	0.01067	0.00952	2.54000	0.45200	0.51000	-10.7
9	0.01148	0.01138	2.40500	0.52400	0.57200	-0.9
10	0.00137	0.00131	0.48900	0.09800	0.51300	-4.8
11	0.00400	0.00493	0.48000	0.48000	2.55000	23.4
12	0.00342	0.00227	0.55500	0.29900	1.64500	-33.5
13	0.00711	0.00671	0.59900	0.99600	0.90700	-5.6
14	0.00624	0.00539	0.43800	1.52300	0.13600	-13.6
15	0.00666	0.00713	0.47800	1.48000	0.14400	6.9

PHI = 0.000017
 AVG PCT ERROR = 14.4

// JOB F 1001 2002 3003 4004 F 2002

FU

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - LSEST GROUP - CSRD

// FOR

*ONE WORD INTEGERS

*LIST ALL

```

SUBROUTINE FUN(BB)
DIMENSION BB(10)
COMMON KEY,MJM,ND,NF,NFD,NI,NP,PHIZ,SL,B(10),F( 40),G(10),S(10),
1 Y( 40),A(10,10),X(40,16),P(1,10),IPRIN,ILM,MAT,MAR,IPART,
2 FF( 40),KPOIN,NR,NW
DO 1 I=1,ND
DENOM = 1+(BB(1)*X(I,1))**.5 + BB(2)*X(I,2) + BB(3)*X(I,3)
1 FF(I) =BB(1)*BB(2)* BB(4)*X(I,1)*X(I,2) / DENOM**3
RETURN
END

```

VARIABLE ALLOCATIONS

KEY(IC)=7FFF	MJM(IC)=7FFE	ND(IC)=7FFD	NF(IC)=7FF
NP(IC)=7FF9	PHIZ(RC)=7FF6	SL(RC)=7FF4	B(RC)=7FF
S(RC)=7F7A-7F68	Y(RC)=7F66-7F18	A(RC)=7F16-7E50	X(RC)=7E4
ILM(IC)=793A	MAT(IC)=7939	MAR(IC)=7938	IPART(IC)=793
NR(IC)=78E4	NW(IC)=78E3	DENOM(R)=0000	I(I)=000

STATEMENT ALLOCATIONS

1 =005D

FEATURES SUPPORTED

ONE WORD INTEGERS

CALLED SUBPROGRAMS

FAXB	FADD	FMPYX	FLD	FLDX	FSTO	FSTOX	FDVR	FAXI	F
------	------	-------	-----	------	------	-------	------	------	---

REAL CONSTANTS

.500000E 00=0010

INTEGER CONSTANTS

1=0012 3=0013

CORE REQUIREMENTS FOR FUN

COMMON 1822 VARIABLES 16 PROGRAM 120

RELATIVE ENTRY POINT ADDRESS IS 0014 (HEX)

END OF COMPILATION

// DUP

*DELETE	FUN	2002
CART ID 2002	DB ADDR 3F6B	DB CNT 0009

*STORE	WS	UA	FUN	2002	2002
CART ID 2002	DB ADDR 3F7D	DB CNT 000A			

// JOB F 1001 2002 3003 4004 F 2002

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - LSEST GROUP - CSRD

// FOR

*ONE WORD INTEGERS

*LIST ALL

SUBROUTINE PART

COMMON KEY, MJM, ND, NF, NFD, NI, NP, PHIZ, SL, B(10), F(40), G(10), S(10),
1 Y(40), A(10,10), X(40,16), P(1,10), IPRIN, ILM, MAT, MAR, IPART,

2 FF(40), KPOIN, NR, NW

1 K=KPOIN

DENOM = 1. + (B(1)*X(K,1))**0.5 + B(2)*X(K,2) + B(3)*X(K,3)

P(1,1)= B(2)*B(4)*X(K,1)*X(K,2)*(DENOM-1.5*B(1)**0.5*X(K,1)**0.5)
/ DENOM**4

1 P(1,2)= B(1)*B(4)*X(K,1)*X(K,2)*(DENOM-3.0*B(2)*X(K,2)) /DENOM**4

P(1,3)= 3.0*B(1)*B(2)*B(4)*X(K,1)*X(K,2)*X(K,3) / DENOM**4

P(1,4)= B(1)*B(2)*X(K,1)*X(K,2) / DENOM**3

RETURN

END

VARIABLE ALLOCATIONS

KEY(IC)=7FFF

NP(IC)=7FF9

S(RC)=7F7A-7F68

ILM(IC)=793A

NR(IC)=78E4

MJM(IC)=7FFE

PHIZ(RC)=7FF6

Y(RC)=7F66-7F18

MAT(IC)=7939

NW(IC)=78E3

ND(IC)=7FFD

SL(RC)=7FF4

A(RC)=7F16-7E50

MAR(IC)=7938

DENOM(R)=0000

NF(IC)=7FFC

B(RC)=7FF2

X(RC)=7E4E

IPART(IC)=7937

K(I)=0008

UNREFERENCED STATEMENTS

1

STATEMENT ALLOCATIONS

1 =001B

FEATURES SUPPORTED

ONE WORD INTEGERS

CALLED SUBPROGRAMS

FAXB FADD FMPY FMPYX FLD FLDX FSTO FSTOX FSBR FD

REAL CONSTANTS

.100000E 01=0010 .500000E 00=0012 .150000E 01=0014 .300000E 01=C

INTEGER CONSTANTS

4=0018 3=0019

CORE REQUIREMENTS FOR PART

COMMON 1822 VARIABLES 16 PROGRAM 236

RELATIVE ENTRY POINT ADDRESS IS 001A (HEX)

END OF COMPILATION

// DUP

*DELETE

CART ID 2002 DB ADDR 3F6B DB CNT 0012

*STORE

WS UA PART 2002 2002
CART ID 2002 DB ADDR 3F75 DB CNT 0012

lsc.

DEPENDENT	INDEPENDENT 1	2	3
0.12330E-02	0.48200E 00	0.10000E 00	0.50800E
0.12142E-01	0.24590E 01	0.52700E 00	0.51500E
0.12393E-01	0.24500E 01	0.53000E 00	0.51500E
0.15100E-02	0.47700E 00	0.49400E 00	0.25380E
0.54950E-02	0.51400E 00	0.54000E 00	0.45500E
0.56130E-02	0.47300E 00	0.55200E 00	0.47300E
0.57520E-02	0.47000E 00	0.55800E 00	0.47300E
0.14360E-02	0.10400E 00	0.56200E 00	0.44000E
0.59870E-02	0.45000E 00	0.28400E 01	0.23000E
0.50470E-02	0.40900E 00	0.28100E 01	0.28900E
0.31060E-02	0.48400E 00	0.10750E 01	0.94200E
0.86460E-02	0.35700E 00	0.15900E 01	0.15300E

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.95964E-05 SQRT(PHI)/ND= 0.25815E-03 LAMBDA= 0.10000E-01
 PARAMETERS 0.33300E 00 0.57600E 00 0.49000E 00 0.73600E

PHI= 0.94616E-05 SQRT(PHI)/ND= 0.25633E-03 LAMBDA= 0.10000E 01
 PARAMETERS 0.34264E 00 0.57114E 00 0.47037E 00 0.74491E

PHI= 0.94616E-05 SQRT(PHI)/ND= 0.25633E-03 LAMBDA= 0.99999E-01
 PARAMETERS 0.34264E 00 0.57114E 00 0.47037E 00 0.74491E

ALGORITHM TERMINATED

PHI= 0.94616E-05 SQRT(PHI)/ND= 0.25633E-03 LAMBDA= 0.10000E 04
 PARAMETERS 0.34264E 00 0.57114E 00 0.47037E 00 0.74491E

SINGULAR MATRIX

DEPENDENT	DIFFERENCE	INDEPENDENT 1	2	3
0.14240E-02	-0.19101E-03	0.48200E 00	0.10000E 00	0.50800E
0.12672E-01	-0.53020E-03	0.24590E 01	0.52700E 00	0.51500E
0.12697E-01	-0.30419E-03	0.24500E 01	0.53000E 00	0.51500E
0.14376E-02	0.72338E-04	0.47700E 00	0.49400E 00	0.25380E
0.55237E-02	-0.28768E-04	0.51400E 00	0.54000E 00	0.45500E
0.52103E-02	0.40269E-03	0.47300E 00	0.55200E 00	0.47300E
0.52161E-02	0.53580E-03	0.47000E 00	0.55800E 00	0.47300E
0.16840E-02	-0.24809E-03	0.10400E 00	0.56200E 00	0.44000E
0.61171E-02	-0.13019E-03	0.45000E 00	0.28400E 01	0.23000E
0.55420E-02	-0.49500E-03	0.40900E 00	0.28100E 01	0.28900E
0.50683E-02	-0.19623E-02	0.48400E 00	0.10750E 01	0.94200E
0.65431E-02	0.21028E-02	0.35700E 00	0.15900E 01	0.15300E

CORRELATION MATRIX

1.000				
0.495	1.000			
0.863	0.805	1.000		
0.964	0.681	0.923	1.000	

3 STEPS

DEPENDENT	INDEPENDENT		
	1	2	3
0.26610E-02	0.47800E 00	0.10200E 00	0.52500E 00
0.17506E-01	0.25050E 01	0.51800E 00	0.49700E 00
0.17206E-01	0.25000E 01	0.51700E 00	0.48500E 00
0.52860E-02	0.42500E 00	0.27700E 01	0.31000E 00
0.49170E-02	0.43300E 00	0.28000E 01	0.27000E 00
0.62520E-02	0.48900E 00	0.56200E 00	0.51000E 00
0.41120E-02	0.54600E 00	0.50600E 00	0.44600E 00
0.69200E-02	0.46900E 00	0.55600E 00	0.47500E 00
0.19150E-02	0.10000E 00	0.54000E 00	0.46400E 00
0.24370E-02	0.42200E 00	0.46200E 00	0.26150E 00
0.30040E-02	0.46700E 00	0.48500E 00	0.25550E 00
0.11106E-01	0.14950E 01	0.51100E 00	0.49500E 00
0.17476E-01	0.12220E 01	0.77600E 00	0.10300E 00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.18162E-04 PARAMETERS	SQRT(PHI)/ND= 0.32783E-03 0.18700E 00	0.61700E 00	LAMBDA= 0.10000E-01 0.20500E 00	0.10510E 01
PHI= 0.18061E-04 PARAMETERS	SQRT(PHI)/ND= 0.32691E-03 0.18741E 00	0.61746E 00	LAMBDA= 0.10000E 02 0.20428E 00	0.10526E 01
PHI= 0.18008E-04 PARAMETERS	SQRT(PHI)/ND= 0.32643E-03 0.18774E 00	0.61763E 00	LAMBDA= 0.99999E 01 0.20325E 00	0.10540E 01
PHI= 0.17990E-04 PARAMETERS	SQRT(PHI)/ND= 0.32627E-03 0.18800E 00	0.61756E 00	LAMBDA= 0.99999E 01 0.20196E 00	0.10551E 01
PHI= 0.17990E-04 PARAMETERS	SQRT(PHI)/ND= 0.32627E-03 0.18800E 00	0.61756E 00	LAMBDA= 0.99999E-01 0.20196E 00	0.10551E 01
PHI= 0.17990E-04 PARAMETERS	SQRT(PHI)/ND= 0.32626E-03 0.18801E 00	0.61756E 00	LAMBDA= 0.99999E-01 0.20197E 00	0.10551E 01
PHI= 0.17989E-04 PARAMETERS	SQRT(PHI)/ND= 0.32626E-03 0.18801E 00	0.61756E 00	LAMBDA= 0.99999E-01 0.20197E 00	0.10551E 01
PHI= 0.17989E-04 PARAMETERS	SQRT(PHI)/ND= 0.32626E-03 0.18802E 00	0.61756E 00	LAMBDA= 0.99999E-01 0.20197E 00	0.10551E 01
PHI= 0.17989E-04 PARAMETERS	SQRT(PHI)/ND= 0.32625E-03 0.18803E 00	0.61756E 00	LAMBDA= 0.99999E-01 0.20197E 00	0.10551E 01
PHI= 0.17989E-04 PARAMETERS	SQRT(PHI)/ND= 0.32625E-03 0.18803E 00	0.61755E 00	LAMBDA= 0.99999E-01 0.20197E 00	0.10551E 01
PHI= 0.17989E-04 PARAMETERS	SQRT(PHI)/ND= 0.32625E-03 0.18803E 00	0.61755E 00	LAMBDA= 0.99999E 03 0.20196E 00	0.10551E 01
PHI= 0.17988E-04 PARAMETERS	SQRT(PHI)/ND= 0.32625E-03 0.18803E 00	0.61755E 00	LAMBDA= 0.99999E-01 0.20196E 00	0.10551E 01
PHI= 0.17988E-04 PARAMETERS	SQRT(PHI)/ND= 0.32625E-03 0.18804E 00	0.61755E 00	LAMBDA= 0.99999E-01 0.20196E 00	0.10551E 01
PHI= 0.17988E-04 PARAMETERS	SQRT(PHI)/ND= 0.32624E-03 0.18805E 00	0.61755E 00	LAMBDA= 0.99999E-01 0.20197E 00	0.10551E 01
PHI= 0.17987E-04 PARAMETERS	SQRT(PHI)/ND= 0.32624E-03 0.18805E 00	0.61755E 00	LAMBDA= 0.99999E-01 0.20197E 00	0.10551E 01
PHI= 0.17987E-04 PARAMETERS	SQRT(PHI)/ND= 0.32624E-03 0.18806E 00	0.61755E 00	LAMBDA= 0.99999E-01 0.20197E 00	0.10551E 01
PHI= 0.17987E-04 PARAMETERS	SQRT(PHI)/ND= 0.32624E-03 0.18806E 00	0.61755E 00	LAMBDA= 0.99999E-01 0.20197E 00	0.10551E 01
PHI= 0.17986E-04 PARAMETERS	SQRT(PHI)/ND= 0.32623E-03 0.18807E 00	0.61755E 00	LAMBDA= 0.99999E-01 0.20197E 00	0.10551E 01
PHI= 0.17986E-04 PARAMETERS	SQRT(PHI)/ND= 0.32623E-03 0.18807E 00	0.61755E 00	LAMBDA= 0.99999E-01 0.20198E 00	0.10551E 01
PHI= 0.17986E-04 PARAMETERS	SQRT(PHI)/ND= 0.32623E-03 0.18808E 00	0.61755E 00	LAMBDA= 0.99999E-01 0.20198E 00	0.10551E 01
PHI= 0.17985E-04	SQRT(PHI)/ND= 0.32622E-03		LAMBDA= 0.99999E-01	

```

PARAMETERS          0.18809E 00    0.61755E 00    0.20198E 00    0.10551E 0
PHI= 0.17985E-04   SQR(T(PHI))/ND= 0.32622E-03    LAMBDA= 0.99999E-01
PARAMETERS          0.18809E 00    0.61755E 00    0.20198E 00    0.10551E 0
PHI= 0.17985E-04   SQR(T(PHI))/ND= 0.32622E-03    LAMBDA= 0.99999E-01
PARAMETERS          0.18810E 00    0.61755E 00    0.20199E 00    0.10551E 0
PHI= 0.17984E-04   SQR(T(PHI))/ND= 0.32622E-03    LAMBDA= 0.99999E-01
PARAMETERS          0.18810E 00    0.61755E 00    0.20199E 00    0.10551E 0
PHI= 0.17984E-04   SQR(T(PHI))/ND= 0.32621E-03    LAMBDA= 0.99999E-01
PARAMETERS          0.18811E 00    0.61755E 00    0.20199E 00    0.10551E 0
PHI= 0.17984E-04   SQR(T(PHI))/ND= 0.32621E-03    LAMBDA= 0.99999E-01
PARAMETERS          0.18811E 00    0.61755E 00    0.20199E 00    0.10551E 0
PHI= 0.17984E-04   SQR(T(PHI))/ND= 0.32621E-03    LAMBDA= 0.99999E 03
PARAMETERS          0.18812E 00    0.61755E 00    0.20198E 00    0.10551E 0
PHI= 0.17984E-04   SQR(T(PHI))/ND= 0.32621E-03    LAMBDA= 0.99999E-01
PARAMETERS          0.18812E 00    0.61755E 00    0.20198E 00    0.10551E 0
PHI= 0.17983E-04   SQR(T(PHI))/ND= 0.32620E-03    LAMBDA= 0.99999E-01
PARAMETERS          0.18813E 00    0.61755E 00    0.20198E 00    0.10551E 0
PHI= 0.23367E-04   SQR(T(PHI))/ND= 0.37184E-03    LAMBDA= 0.99999E-01
PARAMETERS          0.18936E 00    0.60969E 00    0.15602E 00    0.10914E 0

```

ALGORITHM CONVERGED

run was aborted voluntarily

DEPENDENT	DIFFERENCE	INDEPENDENT		
		1	2	3
0.20364E-02	0.62457E-03	0.47800E 00	0.10200E 00	0.52500E 00
0.18115E-01	-0.50804E-03	0.25050E 01	0.51800E 00	0.49700E 00
0.18125E-01	-0.92055E-03	0.25000E 01	0.51700E 00	0.48500E 00
0.53810E-02	-0.95005E-04	0.42500E 00	0.27700E 01	0.31000E 00
0.54615E-02	-0.54451E-03	0.43300E 00	0.28000E 01	0.27000E 00
0.76407E-02	-0.13887E-02	0.48900E 00	0.56200E 00	0.51000E 00
0.70905E-02	-0.29785E-02	0.54600E 00	0.50600E 00	0.44600E 00
0.65587E-02	0.36128E-03	0.46900E 00	0.55600E 00	0.47500E 00
0.18658E-02	0.49118E-04	0.10000E 00	0.54000E 00	0.46400E 00
0.32018E-02	-0.76484E-03	0.42200E 00	0.46200E 00	0.26150E 00
0.36122E-02	-0.60829E-03	0.46700E 00	0.48500E 00	0.25550E 00
0.13582E-01	-0.24766E-02	0.14950E 01	0.51100E 00	0.49500E 00
0.15623E-01	0.18522E-02	0.12220E 01	0.77600E 00	0.10300E 00

CORRELATION MATRIX

1.000			
0.773	1.000		
0.790	0.809	1.000	
0.986	0.849	0.811	1.000

28 STEPS

DEPENDENT	INDEPENDENT		2	3
	1			
0.59270E-02	0.50000E 00	0.27350E 01	0.27000E 01	0.27000E 01
0.47730E-02	0.48200E 00	0.56000E 00	0.62000E 01	0.62000E 01
0.44520E-02	0.50100E 00	0.53300E 00	0.46600E 01	0.46600E 01
0.60520E-02	0.47500E 00	0.55300E 00	0.47100E 01	0.47100E 01
0.74050E-02	0.47600E 00	0.55600E 00	0.47800E 01	0.47800E 01
0.16620E-02	0.10100E 00	0.54800E 00	0.45100E 01	0.45100E 01
0.14027E-01	0.23350E 01	0.55000E 00	0.61000E 01	0.61000E 01
0.95280E-02	0.25400E 01	0.45200E 00	0.51000E 01	0.51000E 01
0.11381E-01	0.24050E 01	0.52400E 00	0.57200E 01	0.57200E 01
0.13120E-02	0.48900E 00	0.98000E-01	0.51300E 01	0.51300E 01
0.49380E-02	0.48000E 00	0.48000E 00	0.25500E 01	0.25500E 01
0.22770E-02	0.55500E 00	0.29900E 00	0.16450E 01	0.16450E 01
0.67180E-02	0.59900E 00	0.99600E 00	0.90700E 01	0.90700E 01
0.53950E-02	0.43800E 00	0.15230E 01	0.13600E 01	0.13600E 01
0.71320E-02	0.47800E 00	0.14800E 01	0.14400E 01	0.14400E 01

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.17588E-04 PARAMETERS	SQRT(PHI)/ND= 0.27958E-03 0.30200E 00	0.48800E 00	LAMBDA= 0.10000E-01 0.41000E-01	0.59900E 01
PHI= 0.17354E-04 PARAMETERS	SQRT(PHI)/ND= 0.27772E-03 0.30453E 00	0.49584E 00	LAMBDA= 0.10000E 01 0.50102E-01	0.60207E 01
PHI= 0.17322E-04 PARAMETERS	SQRT(PHI)/ND= 0.27746E-03 0.30528E 00	0.49745E 00	LAMBDA= 0.10000E 02 0.52326E-01	0.60293E 01
PHI= 0.17310E-04 PARAMETERS	SQRT(PHI)/ND= 0.27737E-03 0.30594E 00	0.49892E 00	LAMBDA= 0.99999E 01 0.54496E-01	0.60368E 01
PHI= 0.17309E-04 PARAMETERS	SQRT(PHI)/ND= 0.27736E-03 0.30602E 00	0.49909E 00	LAMBDA= 0.99999E 02 0.54752E-01	0.60377E 01
PHI= 0.17308E-04 PARAMETERS	SQRT(PHI)/ND= 0.27735E-03 0.30610E 00	0.49926E 00	LAMBDA= 0.99999E 02 0.55006E-01	0.60386E 01
PHI= 0.17307E-04 PARAMETERS	SQRT(PHI)/ND= 0.27735E-03 0.30618E 00	0.49943E 00	LAMBDA= 0.99999E 02 0.55260E-01	0.60395E 01
PHI= 0.17307E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30625E 00	0.49960E 00	LAMBDA= 0.99999E 02 0.55512E-01	0.60404E 01
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30633E 00	0.49976E 00	LAMBDA= 0.99999E 02 0.55764E-01	0.60413E 01
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30640E 00	0.49993E 00	LAMBDA= 0.99999E 02 0.56016E-01	0.60421E 01
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30641E 00	0.49993E 00	LAMBDA= 0.99999E-01 0.56016E-01	0.60421E 01
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30641E 00	0.49994E 00	LAMBDA= 0.99999E 03 0.56041E-01	0.60422E 01
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30642E 00	0.49996E 00	LAMBDA= 0.99999E 03 0.56067E-01	0.60423E 01
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30643E 00	0.49998E 00	LAMBDA= 0.99999E 03 0.56092E-01	0.60424E 01
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30643E 00	0.49998E 00	LAMBDA= 0.99999E-01 0.56092E-01	0.60424E 01
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30643E 00	0.49998E 00	LAMBDA= 0.99999E-01 0.56092E-01	0.60424E 01
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30644E 00	0.49999E 00	LAMBDA= 0.99999E 03 0.56118E-01	0.60425E 01
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30644E 00	0.49999E 00	LAMBDA= 0.99999E-01 0.56117E-01	0.60425E 01
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30644E 00	0.49999E 00	LAMBDA= 0.99999E-01 0.56117E-01	0.60425E 01

PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27734E-03 0.30644E 00	0.49999E 00	LAMBDA= 0.99999E-01 0.56117E-01	0.60425E 00
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27733E-03 0.30645E 00	0.50001E 00	LAMBDA= 0.99999E 03 0.56142E-01	0.60425E 00
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27733E-03 0.30645E 00	0.50001E 00	LAMBDA= 0.10000E 04 0.56142E-01	0.60425E 00
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27733E-03 0.30645E 00	0.50001E 00	LAMBDA= 0.99999E-01 0.56142E-01	0.60425E 00
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27733E-03 0.30646E 00	0.50003E 00	LAMBDA= 0.99999E 03 0.56168E-01	0.60426E 00
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27733E-03 0.30646E 00	0.50003E 00	LAMBDA= 0.99999E-01 0.56167E-01	0.60426E 00
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27733E-03 0.30646E 00	0.50003E 00	LAMBDA= 0.99999E-01 0.56167E-01	0.60426E 00
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27733E-03 0.30647E 00	0.50004E 00	LAMBDA= 0.99999E 03 0.56193E-01	0.60427E 00
PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27733E-03 0.30647E 00	0.50004E 00	LAMBDA= 0.10000E 04 0.56193E-01	0.60427E 00

ALGORITHM TERMINATED

PHI= 0.17306E-04 PARAMETERS	SQRT(PHI)/ND= 0.27733E-03 0.30647E 00	0.50004E 00	LAMBDA= 0.10000E 04 0.56193E-01	0.60427E 00
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SINGULAR MATRIX

DEPENDENT	DIFFERENCE	INDEPENDENT	2	3
		1		
0.59309E-02	-0.39646E-05	0.50000E 00	0.27350E 01	0.27000E 00
0.53876E-02	-0.61464E-03	0.48200E 00	0.56000E 00	0.62000E-01
0.51730E-02	-0.72103E-03	0.50100E 00	0.53300E 00	0.46600E 00
0.50888E-02	0.96319E-03	0.47500E 00	0.55300E 00	0.47100E 00
0.51062E-02	0.22987E-02	0.47600E 00	0.55600E 00	0.47800E 00
0.15962E-02	0.65777E-04	0.10100E 00	0.54800E 00	0.45100E 00
0.11879E-01	0.21474E-02	0.23350E 01	0.55000E 00	0.61000E 00
0.10894E-01	-0.13666E-02	0.25400E 01	0.45200E 00	0.51000E 00
0.11698E-01	-0.31770E-03	0.24050E 01	0.52400E 00	0.57200E 00
0.14115E-02	-0.99558E-04	0.48900E 00	0.98000E-01	0.51300E 00
0.38682E-02	0.10697E-02	0.48000E 00	0.48000E 00	0.25500E 01
0.33939E-02	-0.11169E-02	0.55500E 00	0.29900E 00	0.16450E 01
0.71448E-02	-0.42682E-03	0.59900E 00	0.99600E 00	0.90700E 00
0.63424E-02	-0.94741E-03	0.43800E 00	0.15230E 01	0.13600E 00
0.67707E-02	0.36129E-03	0.47800E 00	0.14800E 01	0.14400E 00

CORRELATION MATRIX

1.000			
0.659	1.000		
0.742	0.756	1.000	
0.961	0.818	0.778	1.000

28 STEPS

```
PAGE 1 02/06/73
// JOB F 1001 2002 3003 4004 F 2002
LOG DRIVE CART SPEC CART AVAIL PHY DRIVE
0000 000F 000F 0000
0001 1001 1001 0001
0002 2002 2002 0002
0003 3003 3003 0003
0004 4004 4004 0004
```

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - SYNT GROUP - CSRD

```
// FOR
*ONE WORD INTEGERS
*LIST ALL
*IOCS(CARD,1403 PRINTER)
C HYDROGENATION OF CODIMER
C PROGRAM TO CALC ERROR AFTER FINDING CONSTANTS
C MECHANISM - DISSOCIATION OF HYDROGEN
C
C REAL KH,KU,KS
C DIMENSION PH(20),PU(20),PS(20),REXP(20),RCALC(20),DIFF(20)
C
C ICRD=2
C LPRT=5
C PHI=0.0
C ERROR = 0.0
C
C *** READ CONSTANTS ***
C
C READ(ICRD,100) KH,KU,KS,EK
C
C L=0
C 2 L=L+1
C READ(ICRD,102) REXP(L),PH(L),PU(L),PS(L)
C IF( PH(L) ) 60,30,20
C 20 DENOM = 1 + (KH*PH(L))*0.5 + KU*PU(L) + KS*PS(L)
C RCALC(L) = EK*KH*KU*PH(L)*PU(L) / DENOM**3
C DIFF(L) = ( REXP(L) - RCALC(L) ) / RCALC(L) * 100.
C PHI = PHI + ( RCALC(L) - REXP(L) )**2
C GO TO 2
C 30 KOUNT = L-1
C WRITE(LPRT,110)
C WRITE(LPRT,111) KH
C WRITE(LPRT,112) KU
C WRITE(LPRT,113) KS
C WRITE(LPRT,114) EK
C WRITE(LPRT,120)
C DO 50 L = 1,KOUNT
C ERROR = ERROR + ABS(DIFF(L))
C 50 WRITE(LPRT,130) L,RCALC(L),REXP(L),PH(L),PU(L),PS(L),DIFF(L)
C XNUM=KOUNT
C ERROR = ERROR / XNUM
C WRITE(LPRT,140) PHI, ERROR
C 60 CALL EXIT
C
C 100 FORMAT( 4F15.0 )
C 102 FORMAT( 10X,4F10.0 )
C 110 FORMAT( 1H1 )
C 111 FORMAT( 6H KH = , F6.4 )
C 112 FORMAT( 6H KU = , F6.4 )
C 113 FORMAT( 6H KS = , F6.4 )
C 114 FORMAT( 6H EK = , F6.4 / )
C 120 FORMAT(3X,50H CALC EXPER PH PU PS
C 1 3X,20H RXN RATE RXN RATE ,35X,10H PCT ERROR )
C 130 FORMAT(1X,12,5F10.5,F10.1 )
C 140 FORMAT( // 18H PHI = , F10.6
C 1 / 18H AVG PCT ERROR = , F10.1 )
C
C END
C
C VARIABLE ALLOCATIONS
C PH(R )=0026-0000 PU(R )=004E-0028 PS(R )=0076-0050 REXP(R )=009
C KH(R )=00F0 KU(R )=00F2 KS(R )=00F4 PHI(R )=00F
C DENOM(R )=00FC XNUM(R )=00FE ICRD(I )=0106 LPRT(I )=010
C
C STATEMENT ALLOCATIONS
C 100 =0117 102 =011A 110 =011E 111 =0121 112 =0127 113 =012D 1
C 2 =01C0 20 =01DF 30 =0234 50 =026F 60 =029F
```

KH = 0.3430
 KU = 0.5710
 KS = 0.4700
 EK = 0.7450

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00142	0.00123	0.48200	0.10000	0.50800	-13.4
2	0.01268	0.01214	2.45900	0.52700	0.51500	-4.2
3	0.01270	0.01239	2.45000	0.53000	0.51500	-2.4
4	0.00144	0.00151	0.47700	0.49400	2.53800	4.8
5	0.00552	0.00549	0.51400	0.54000	0.45500	-0.6
6	0.00521	0.00561	0.47300	0.55200	0.47300	7.6
7	0.00522	0.00575	0.47000	0.55800	0.47300	10.1
8	0.00168	0.00143	0.10400	0.56200	0.44000	-14.8
9	0.00612	0.00598	0.45000	2.84000	0.23000	-2.2
10	0.00554	0.00504	0.40900	2.81000	0.28900	-9.0
11	0.00507	0.00310	0.48400	1.07500	0.94200	-38.7
12	0.00654	0.00864	0.35700	1.59000	0.15300	32.0

PHI = 0.000009
 AVG PCT ERROR = 11.6

Synthetic Data with 15% Error - Results of Non-linear Regression
 mechanism(h)

163.

KH = 0.1880
 KU = 0.6180
 KS = 0.2020
 EK = 1.0550

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00188	0.00266	0.47800	0.10200	0.52500	41.1
2	0.01700	0.01750	2.50500	0.51800	0.49700	2.9
3	0.01703	0.01720	2.50000	0.51700	0.48500	1.0
4	0.00505	0.00528	0.42500	2.77000	0.31000	4.6
5	0.00513	0.00491	0.43300	2.80000	0.27000	-4.2
6	0.00735	0.00625	0.48900	0.56200	0.05100	-14.9
7	0.00661	0.00411	0.54600	0.50600	0.44600	-37.8
8	0.00610	0.00692	0.46900	0.55600	0.47500	13.3
9	0.00172	0.00191	0.10000	0.54000	0.46400	10.8
10	0.00259	0.00243	0.42200	0.46200	2.61500	-6.1
11	0.00294	0.00300	0.46700	0.48500	2.55500	1.9
12	0.01270	0.01110	1.49500	0.51100	0.49500	-12.6
13	0.01498	0.01747	1.22200	0.77600	0.10300	16.6

PHI = 0.000017
 AVG PCT ERROR = 12.9

KH = 0.3060
 KU = 0.5000
 KS = 0.0560
 EK = 0.6040

	CALC	EXPER	PH	PU	PS	PCT ERROR
	RXN RATE	RXN RATE				
1	0.00592	0.00592	0.50000	2.73500	0.27000	0.0
2	0.00537	0.00477	0.48200	0.56000	0.06200	-11.2
3	0.00516	0.00445	0.50100	0.53300	0.46600	-13.8
4	0.00508	0.00605	0.47500	0.55300	0.47100	19.0
5	0.00509	0.00740	0.47600	0.55600	0.47800	45.2
6	0.00159	0.00166	0.10100	0.54800	0.45100	4.2
7	0.01186	0.01402	2.33500	0.55000	0.61000	18.1
8	0.01088	0.00952	2.54000	0.45200	0.51000	-12.4
9	0.01168	0.01138	2.40500	0.52400	0.57200	-2.6
10	0.00140	0.00131	0.48900	0.09800	0.51300	-6.9
11	0.00386	0.00493	0.48000	0.48000	2.55000	27.7
12	0.00339	0.00227	0.55500	0.29900	1.64500	-32.8
13	0.00713	0.00671	0.59900	0.99600	0.90700	-5.8
14	0.00633	0.00539	0.43800	1.52300	0.13600	-14.8
15	0.00676	0.00713	0.47800	1.48000	0.14400	5.4

PHI = 0.000017
 AVG PCT ERROR = 14.7

Synthetic Reaction Rates Generated from Equation for molecularly adsorbed H₂
 fitted to equation for molecularly adsorbed H₂
 NO ERROR - 200°C
 DISSOCIATION OF HYDROGEN LINEAR REGRESSION
 mechanism (h)

165.

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.0542
STANDARD ERROR OF THE MEAN	0.0156
MULTIPLE R	0.9958
MULTIPLE RSQR	0.9918

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.35684883	0.02746916	0.9771	0.4412
PH2	0.87943029	0.04499845	0.9896	0.6461
PU	0.54541266	0.01938746	0.9949	0.9817

CONSTANT 1.7456295

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.12456E 03	0.12456E 03	
REGRESSION	3	0.28538E 01	0.95129E 00	0.32309E 0
ERROR	8	0.23554E-01	0.29443E-02	

$a = 1.7456$
 $K_H = \left(\frac{b}{a}\right)^2 = \left(\frac{0.8794}{1.7456}\right)^2 = 0.2538$
 $b = 0.8794$
 $K_U = \frac{c}{a} = \frac{0.5454}{1.7456} = 0.3124$
 $c = 0.5454$
 $K_S = \frac{d}{a} = \frac{0.3568}{1.7456} = 0.2044$
 $d = 0.3568$
 $E_k = \frac{1}{a^3 K_H K_U} = 2.3712$

275°C

DISSOCIATION OF HYDROGEN LINEAR REGRESSION

100.

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.0420
STANDARD ERROR OF THE MEAN	0.0116
*MULTIPLE R	0.9972
MULTIPLE RSQR	0.9945

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.20829388	0.01539190	0.9762	0.3560
PH2	0.56920266	0.03330045	0.9849	0.4450
PU	0.60007333	0.01500096	0.9971	1.0557
CONSTANT	1.8195860			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.11500E 03	0.11500E 03	
REGRESSION	3	0.29101E 01	0.97003E 00	0.54775E 03
ERROR	9	0.15938E-01	0.17709E-02	

$$= 1.8196$$

$$K_H = \left(\frac{b}{a}\right)^2 = \left(\frac{0.5692}{1.8196}\right)^2 = 0.0978$$

$$= 0.5692$$

$$K_U = \frac{c}{a} = \frac{0.6001}{1.8196} = 0.3298$$

$$= 0.6001$$

$$K_S = \frac{d}{a} = \frac{0.2083}{1.8196} = 0.1145$$

$$= 0.2083$$

$$ER = \frac{1}{a^3 K_H K_U} = 5.146$$

DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.0371
STANDARD ERROR OF THE MEAN	0.0095
MULTIPLE R	0.9967
MULTIPLE RSQR	0.9935

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	0.01021767	0.01632732	0.1855	0.0161
PH2	0.59105909	0.02662926	0.9890	0.5481
PU	0.58473682	0.01616745	0.9958	0.9470
CONSTANT	2.1862111			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.14963E 03	0.14963E 03	
REGRESSION	3	0.23430E 01	0.78102E 00	0.56721E 0
ERROR	11	0.15146E-01	0.13769E-02	

$$a = 2.1862 \quad k_H = \left(\frac{b}{a}\right)^2 = \frac{0.5910}{2.1862} = 0.0731$$

$$b = 0.5910 \quad k_U = \frac{c}{a} = \frac{0.5847}{2.1862} = 0.2674$$

$$c = 0.5847 \quad k_S = \frac{d}{a} = \frac{0.0102}{2.1862} = 0.0047$$

$$d = 0.0102 \quad ER = \frac{1}{a^3 k_U k_S} = 4.896$$

DATA FROM MECHANISM (d)

FITTED TO MECHANISM (h)

// JOB F 1001 2002 3003 4004 F 2002

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - SYNT GROUP - CSRD

```

// FOR
*ONE WORD INTEGERS
*LIST ALL
*IOCS(CARD,1403 PRINTER)
C HYDROGENATION OF CODIMER
C PROGRAM TO CALC ERROR AFTER FINDING CONSTANTS
C MECHANISM - DISSOCIATION OF HYDROGEN
C
REAL KH,KU,KS
DIMENSION PH(20),PU(20),PS(20),REXP(20),RCALC(20),DIFF(20)
C
ICRD=2
LPRT=5
PHI=0.0
ERROR = 0.0
C
**** READ CONSTANTS ***
C
READ(ICRD,100) KH,KU,KS,EK
C
L=0
2 L=L+1
READ(ICRD,102) REXP(L),PH(L),PU(L),PS(L)
IF( PH(L) ) 60,30,20
20 DENOM = 1 + (KH*PH(L))*0.5 + KU*PU(L) + KS*PS(L)
RCALC(L) = EK*KH*KU*PH(L)*PU(L) / DENOM**3
DIFF(L) = ( REXP(L) - RCALC(L) ) / RCALC(L) * 100.
PHI = PHI + ( RCALC(L) - REXP(L) )**2
GO TO 2
30 KOUNT = L-1
WRITE(LPRT,110)
WRITE(LPRT,111) KH
WRITE(LPRT,112) KU
WRITE(LPRT,113) KS
WRITE(LPRT,114) EK
WRITE(LPRT,120)
DO 50 L = 1,KOUNT
ERROR = ERROR + ABS(DIFF(L))
50 WRITE(LPRT,130) L,RCALC(L),REXP(L),PH(L),PU(L),PS(L),DIFF(L)
XNUM=KOUNT
ERROR = ERROR / XNUM
WRITE(LPRT,140) PHI, ERROR
60 CALL EXIT
C
100 FORMAT( 4F15.0 )
110 FORMAT( 1H1 )
102 FORMAT( 10X,4F10.0 )
111 FORMAT( 6H KH = , F6.4 )
112 FORMAT( 6H KU = , F6.4 )
113 FORMAT( 6H KS = , F6.4 )
114 FORMAT( 6H EK = , F6.4 / )
120 FORMAT(3X,50H CALC EXPER PH PU PS
1 3X,20H RXN RATE RXN RATE ,35X,10H PCT ERROR )
130 FORMAT(1X,I2,5F10.5,F10.1 )
140 FORMAT( // 18H PHI = , F10.6
1 / 18H AVG PCT ERROR = , F10.1 )
END
VARIABLE ALLOCATIONS
PH(R )=0026-0000 PU(R )=004E-0028 PS(R )=0076-0050 REXP(R )=00
KH(R )=00F0 KU(R )=00F2 KS(R )=00F4 PHI(R )=00
DENOM(R )=00FC XNUM(R )=00FE ICRD(I )=0106 LPRT(I )=01
STATEMENT ALLOCATIONS
100 =0117 110 =011A 102 =011D 111 =0121 112 =0127 113 =012D
2 =01C0 20 =01DF 30 =0234 50 =026F 60 =029F

```

No EXYOR - 200°C

Fitted to equation for atomically adsorbed H₂

169.

KH = 0.2540
KU = 0.3120
KS = 0.2040
EK = 2.3710

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00276	0.00303	0.48200	0.10000	0.50800	9.7
2	0.02786	0.02733	2.45900	0.52700	0.51500	-1.8
3	0.02793	0.02743	2.45000	0.53000	0.51500	-1.8
4	0.00537	0.00534	0.47700	0.49400	2.53800	-0.5
5	0.01220	0.01195	0.51400	0.54000	0.45500	-2.1
6	0.01163	0.01219	0.47300	0.55200	0.47300	4.7
7	0.01167	0.01221	0.47000	0.55800	0.47300	4.6
8	0.00377	0.00332	0.10400	0.56200	0.44000	-11.8
9	0.02049	0.02074	0.45000	2.84000	0.23000	1.1
10	0.01875	0.01880	0.40900	2.81000	0.28900	0.2
11	0.01475	0.01487	0.48400	1.07500	0.94200	0.7
12	0.01744	0.01712	0.35700	1.59000	0.15300	-1.8

PHI. = 0.000001
AVG PCT ERROR = 3.4

Applicable Reaction rates (Generated From mechanism (d)) - 275°C
 Results of fitting to mechanism (h) - 275°C

176.

KH = 0.0978
 KU = 0.3298
 KS = 0.1145
 EK = 5.1460

	CALC	EXPER	PH	PU	PS	PCT ERROR
	RXN RATE	RXN RATE				
1	0.00360	0.00382	0.47800	0.10200	0.52500	6.2
2	0.04212	0.04071	2.50500	0.51800	0.49700	-3.3
3	0.04212	0.04072	2.50000	0.51700	0.48500	-3.3
4	0.01958	0.01961	0.42500	2.77000	0.31000	0.1
5	0.01996	0.02002	0.43300	2.80000	0.27000	0.3
6	0.01627	0.01657	0.48900	0.56200	0.05100	1.8
7	0.01507	0.01543	0.54600	0.50600	0.44600	2.3
8	0.01414	0.01427	0.46900	0.55600	0.47500	0.9
9	0.00380	0.00340	0.10000	0.54000	0.46400	-10.7
10	0.00713	0.00714	0.42200	0.46200	2.61500	0.0
11	0.00812	0.00818	0.46700	0.48500	2.55500	0.7
12	0.03052	0.03146	1.49500	0.51100	0.49500	3.0
13	0.03747	0.03856	1.22200	0.77600	0.10300	2.8

PHI = 0.000006
 AVG PCT ERROR = 2.7

Synthetic Reaction Rates generated by mechanism (1) - NORWAY
 Results of Fitting to mechanism (h) - 325°C

KH = 0.0731
 KU = 0.2674
 KS = 0.0047
 EK = 4.8960

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.01838	0.01866	0.50000	2.73500	0.27000	1.5
2	0.01079	0.01103	0.48200	0.56000	0.06200	2.3
3	0.01071	0.01093	0.50100	0.53300	0.46600	2.0
4	0.01053	0.01069	0.47500	0.55300	0.47100	1.5
5	0.01058	0.01075	0.47600	0.55600	0.47800	1.5
6	0.00281	0.00254	0.10100	0.54800	0.45100	-9.7
7	0.03218	0.03194	2.33500	0.55000	0.61000	-0.7
8	0.02926	0.02870	2.54000	0.45200	0.51000	-1.9
9	0.03164	0.03128	2.40500	0.52400	0.57200	-1.1
10	0.00254	0.00269	0.48900	0.09800	0.51300	6.0
11	0.00942	0.00930	0.48000	0.48000	2.55000	-1.2
12	0.00741	0.00760	0.55500	0.29900	1.64500	2.5
13	0.01761	0.01769	0.59900	0.99600	0.90700	0.4
14	0.01597	0.01576	0.43800	1.52300	0.13600	-1.3
15	0.01705	0.01692	0.47800	1.48000	0.14400	-0.7

PHI = 0.000000
 AVG PCT ERROR = 2.3

EXPONENTIAL FORM OF EQUATION

DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.2237
STANDARD ERROR OF THE MEAN	0.0645
MULTIPLE R	0.9607
MULTIPLE RSQR	0.9230

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	-0.23478114	0.10806377	-0.6091	-0.2382
PH2	0.59716785	0.08190923	0.9322	0.7243
PU	0.46934062	0.08336043	0.8935	0.6183
CONSTANT	-4.0608339			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.23466E 03	0.23466E 03	
REGRESSION	3	0.48045E 01	0.16015E 01	0.31985E 01
ERROR	8	0.40055E 00	0.50069E-01	

$\ln a = \dots - 4.0608$

$a = 0.0172$

DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.3394
STANDARD ERROR OF THE MEAN	0.0941
MULTIPLE R	0.9348
MULTIPLE RSQR	0.8739

VARIABLE ENTERED

PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	-0.17907837	0.09659071	-0.5257	-0.2290
PH2	0.70377910	0.11325112	0.9005	0.7431
PU	0.48278760	0.12385591	0.7924	0.4805
CONSTANT	-3.7627625			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN REGRESSION	1	0.22670E 03	0.22670E 03	0.20798E 0
REGRESSION	3	0.71889E 01	0.23963E 01	
ERROR	9	0.10369E 01	0.11521E 00	

$\ln a = -3.7627$

$a = 0.0232$

Polynomial equation - 3250

DISSOCIATION OF HYDROGEN LINEAR REGRESSION

REGRESSION ANALYSIS

DEPENDENT VARIABLE	RR
RESIDUAL STANDARD DEVIATION	0.1973
STANDARD ERROR OF THE MEAN	0.0509
MULTIPLE R	0.9711
MULTIPLE RSQR	0.9430

VARIABLE ENTERED PS

VARIABLE	B - COEF	STD ERROR OF B	PARTIAL-R	BETA-COEF
PS	-0.02080489	0.06195684	-0.1007	-0.0265
PH2	0.77155840	0.06474454	0.9633	0.8666
PU	0.49443602	0.07537931	0.8924	0.5161
CONSTANT	-3.7978639			

ANALYSIS OF VARIANCE TABLE

SOURCE	D.F.	SUM OF SQUARES	MEAN SQUARE	F
MEAN	1	0.29113E 03	0.29113E 03	
REGRESSION	3	0.70977E 01	0.23659E 01	0.60751E 02
ERROR	11	0.42838E 00	0.38944E-01	

$\ln a = -3.7978$ $a = 0.0224$

// JOB F 1001 2002 3003 4004 F 2002

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - SYNT GROUP - CSRD

```

// FOR
*ONE WORD INTEGERS
*LIST ALL
*LOCS(CARD,1403 PRINTER)
C HYDROGENATION OF CODIMER
C PROGRAM TO CALC ERROR AFTER FINDING CONSTANTS
C EXPONENTIAL EQUATION
C DIMENSION PH(20),PU(20),PS(20),REXP(20),RCALC(20),DIFF(20)

```

```

C ICRD=2
C LPRT=5
C PHI=0.0
C ERROR = 0.0

```

C *** READ CONSTANTS ***

C READ(ICRD,100) EK,A,B,C

```

C L=0
C 2 L=L+1
C READ(ICRD,102) REXP(L),PH(L),PU(L),PS(L)
C IF( PH(L) ) 60,30,20
C 20 RCALC(L) = EK*PH(L)**A*PU(L)**B*PS(L)**C
C DIFF(L) = ( REXP(L) - RCALC(L) ) / RCALC(L) * 100.
C PHI = PHI + ( RCALC(L) - REXP(L) ) **2

```

```

C 30 GC TO 2
C KOUNT = L-1
C WRITE(LPRT,110)
C WRITE(LPRT,111) EK
C WRITE(LPRT,112) A
C WRITE(LPRT,113) B
C WRITE(LPRT,114) C
C WRITE(LPRT,120)
C DC 50 L = 1, KOUNT
C ERROR = ERROR + ABS(DIFF(L))
C 50 WRITE(LPRT,130) L,RCALC(L),REXP(L),PH(L),PU(L),PS(L),DIFF(L)
C XNUM=KOUNT
C ERROR = ERROR / XNUM
C WRITE(LPRT,140) PHI, ERROR
C 60 CALL EXIT

```

```

C 100 FCRMAT( 4F15.0 )
C 110 FCRMAT( 1H1 )
C 102 FCRMAT( 10X,4F10.0 )
C 111 FCRMAT( 6H EK = , F6.4 )
C 112 FCRMAT( 6H A = , F6.4 )
C 113 FCRMAT( 6H B = , F6.4 )
C 114 FCRMAT( 6H C = , F6.4 / )
C 120 FCRMAT( 3X,50H CALC EXPER PH PU PS
C 1 3X,20H RXN RATE RXN RATE ,35X,10H PCT ERROR )
C 130 FCRMAT( 1X,12,5F10.5,F10.1 )
C 140 FCRMAT( // 18H PHI = , F10.6
C 1 / 18H AVG PCT ERROR = , F10.1 )

```

```

END
VARIABLE ALLOCATIONS
PH(R )=C026-00C0 PU(R )=004E-0028 PS(R )=0076-0050 REXP(R )=009E-007
PHI(R )=C0F0 ERROR(R )=00F2 EK(R )=00F4 A(R )=00F6
XNUM(R )=C0FC ICRD(I )=0102 LPRT(I )=0103 L(I )=0104

```

```

STATEMENT ALLOCATIONS
100 =C110 110 =0113 102 =0116 111 =011A 112 =0120 113 =0126 114 =
2 =01B9 20 =01D8 30 =0212 50 =024D 60 =027D

```

FEATURES SUPPORTED

Exponential Equation - Experimental Data - 200°C

Results of Linear Regression

EK = 0.0172
 A = 0.5970
 B = 0.4690
 C = ***** -0.2348

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00443	0.00353	0.48200	0.10000	0.50800	-20.3
2	0.02547	0.02500	2.45900	0.52700	0.51500	-1.8
3	0.02548	0.03200	2.45000	0.53000	0.51500	25.5
4	0.00638	0.00553	0.47700	0.49400	2.53800	-13.3
5	0.01041	0.00870	0.51400	0.54000	0.45500	-16.5
6	0.00992	0.01392	0.47300	0.55200	0.47300	40.2
7	0.00993	0.00960	0.47000	0.55800	0.47300	-3.4
8	0.00412	0.00514	0.10400	0.56200	0.44000	24.6
9	0.02460	0.01920	0.45000	2.84000	0.23000	-21.9
10	0.02192	0.02060	0.40900	2.81000	0.28900	-6.0
11	0.01170	0.01310	0.48400	1.07500	0.94200	11.9
12	0.01796	0.01860	0.35700	1.59000	0.15300	3.5

PHI = 0.000097
 AVG PCT ERROR = 15.7

check calculation

$$Y = Ek P_H^a P_U^b P_S^c$$

$$Y_1 = (0.0172)(0.482)^{0.597} (0.100)^{0.469} (0.508)^{-0.235}$$

$$= (0.0172)(0.47)(0.340)(1.172) = 0.00443$$

Exponential Equation - Experimental Data - 275°C

Results of Linear Regression

177.

EK = 0.0232
 A = 0.7040
 B = 0.4830
 C = ***** -0.1791

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.00514	0.00298	0.47800	0.10200	0.52500	-42.0
2	0.03652	0.03890	2.50500	0.51800	0.49700	6.4
3	0.03660	0.04500	2.50000	0.51700	0.48500	22.9
4	0.02562	0.02060	0.42500	2.77000	0.31000	-19.6
5	0.02675	0.01850	0.43300	2.80000	0.27000	-30.8
6	0.01808	0.01800	0.48900	0.56200	0.05100	-0.4
7	0.01259	0.01030	0.54600	0.50600	0.44600	-18.2
8	0.01171	0.01215	0.46900	0.55600	0.47500	3.7
9	0.00390	0.00705	0.10000	0.54000	0.46400	80.4
10	0.00732	0.00824	0.42200	0.46200	2.61500	12.4
11	0.00809	0.00734	0.46700	0.48500	2.55500	-9.2
12	0.02525	0.03190	1.49500	0.51100	0.49500	26.3
13	0.03550	0.04350	1.22200	0.77600	0.10300	22.5

PHI = 0.000299
 AVG PCT ERROR = 22.7

EK = 0.0224
 A = 0.7720
 B = 0.4970
 C = ***** -0.0208

Results of Linear Regression

	CALC RXN RATE	EXPER RXN RATE	PH	PU	PS	PCT ERROR
1	0.02222	0.02010	0.50000	2.73500	0.27000	-9.5
2	0.01012	0.01140	0.48200	0.56000	0.06200	12.5
3	0.00976	0.01340	0.50100	0.53300	0.46600	37.2
4	0.00954	0.00946	0.47500	0.55300	0.47100	-0.8
5	0.00957	0.00871	0.47600	0.55600	0.47800	-9.0
6	0.00287	0.00250	0.10100	0.54800	0.45100	-13.1
7	0.03235	0.03380	2.33500	0.55000	0.61000	4.4
8	0.03143	0.02860	2.54000	0.45200	0.51000	-9.0
9	0.03236	0.02970	2.40500	0.52400	0.57200	-8.2
10	0.00412	0.00440	0.48900	0.09800	0.51300	6.7
11	0.00865	0.01106	0.48000	0.48000	2.55500	27.7
12	0.00772	0.00533	0.55500	0.29900	1.64500	-30.9
13	0.01508	0.01885	0.59900	0.99600	0.90700	24.9
14	0.01521	0.01414	0.43800	1.52300	0.13600	-7.0
15	0.01602	0.01590	0.47800	1.48000	0.14400	-0.8

PHI = 0.000064
 AVG PCT ERROR = 13.4

// JOB F 1001 2002 3003 4004 F 2002

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0001	1001	1001	0001
0002	2002	2002	0002
0003	3003	3003	0003
0004	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - LSEST GROUP - CSRD

// FOR

*ONE WORD INTEGERS

*LIST ALL

```

SUBROUTINE FUN(BB)
  DIMENSION BB(10)
  COMMON KEY,MJM,ND,NF,NFD,NI,NP,PHIZ,SL,B(10),F( 40),G(10),S(10),
  1 Y( 40),A(10,10),X(40,16),P(1,10),IPRIN,ILM,MAT,MAR,IPART,
  2 FF( 40),KPOIN,NR,NW
  DO 1 I=1,ND
  1 FF(I) = BB(1)*X(I,1)**BB(2)*X(I,2)**BB(3)*X(I,3)**BB(4)
  RETURN
END

```

VARIABLE ALLOCATIONS

KEY(IC)=7FFF	MJM(IC)=7FFE	ND(IC)=7FFD	NF(IC)
NP(IC)=7FF9	PHIZ(RC)=7FF6	SL(RC)=7FF4	B(RC)
S(RC)=7F7A-7F68	Y(RC)=7F66-7F18	A(RC)=7F16-7E50	X(RC)
ILM(IC)=793A	MAT(IC)=7939	MAR(IC)=7938	IPART(IC)
NR(IC)=78E4	NW(IC)=78E3	I(I)=0004	

STATEMENT ALLOCATIONS

1 =0019

FEATURES SUPPORTED

ONE WORD INTEGERS

CALLED SUBPROGRAMS

FAXBX FMPY FMPYX FLDX FSTO FSTOX SUBSC SUBIN

INTEGER CONSTANTS

1=C00C

CORE REQUIREMENTS FOR FUN

COMMON 1822 VARIABLES 12 PROGRAM 76

RELATIVE ENTRY POINT ADDRESS IS 000D (HEX)

END OF COMPILATION

// DUP

*DELETE		FUN	2002		
CART ID	2002	DB ADDR	2C8B	DB CNT	0006

*STORE	WS	UA	FUN	2002	2002
CART ID	2002	DB ADDR	2D89	DB CNT	0006

// JOB F 1001 2002 3003 4004 F 2002

LOG DRIVE	CART SPEC	CART AVAIL	PHY DRIVE
0000	000F	000F	0000
0C01	1001	1001	0001
CC02	2002	2002	0002
OC03	3003	3003	0003
OC04	4004	4004	0004

V2 M09 ACTUAL 8K CONFIG 8K

USER - WRM PROGRAM NAME - LSEST GROUP - CSRD

```
// FOR
*ONE WORD INTEGERS
*LIST ALL
SUBROUTINE PART
COMMON KEY,MJM,ND,NF,NFD,NI,NP,PHIZ,SL,B(10),F( 40),G(10),S(10),
1 Y( 40),A(10,10),X(40,16),P(1,10),IPRIN,ILM,MAT,MAR,IPART,
2 FF( 40),KPOIN,NR,NW
K=KPOIN
FACT = X(K,1)**B(2)*X(K,2)**B(3)*X(K,3)**B(4)
P(1,1) = FACT
P(1,2) = B(1)*FACT*ALOG(B(2))
P(1,3) = B(1)*FACT*ALOG(B(3))
P(1,4) = B(1)*FACT*ALOG(B(4))
RETURN
END
```

VARIABLE ALLOCATIONS

KEY(IC)=7FFF	MJM(IC)=7FFE	ND(IC)=7FFD	NF(IC)
NP(IC)=7FF9	PHIZ(RC)=7FF6	SL(RC)=7FF4	B(RC)
S(RC)=7F7A-7F68	Y(RC)=7F66-7F18	A(RC)=7F16-7E50	X(RC)
ILM(IC)=793A	MAT(IC)=7939	MAR(IC)=7938	IPART(IC)
NR(IC)=78E4	NW(IC)=78E3	FACT(R)=0000	K(I)

FEATURES SUPPORTED
ONE WORD INTEGERS

CALLED SUBPROGRAMS

FALOG	FAXBX	FMPY	FLD	FLDX	FSTO	FSTOX	SUBSC
-------	-------	------	-----	------	------	-------	-------

CORE REQUIREMENTS FOR PART
COMMON 1822 VARIABLES 18 PROGRAM 132

RELATIVE ENTRY POINT ADDRESS IS 0012 (HEX)

END OF COMPILATION

// DUP

```
*DELETE PART
CART ID 2002 DB ADDR 2C8B DB CNT 000A

*STORE WS UA PART 2002 2002
CART ID 2002 DB ADDR 2D85 DB CNT 000A
```

Exponential expansion

200

181.

DEPENDENT	INDEPENDENT		2	3		
	1					
0.35300E-02	0.48200E	00	0.10000E	00	0.50800E	00
0.25000E-01	0.24590E	01	0.52700E	00	0.51500E	00
0.32000E-01	0.24500E	01	0.53000E	00	0.51500E	00
0.55300E-02	0.47700E	00	0.49400E	00	0.25380E	00
0.87000E-02	0.51400E	00	0.54000E	00	0.45500E	00
0.13920E-01	0.47300E	00	0.55200E	00	0.47300E	00
0.96000E-02	0.47000E	00	0.55800E	00	0.47300E	00
0.51400E-02	0.10400E	00	0.56200E	00	0.44000E	00
0.19200E-01	0.45000E	00	0.28400E	01	0.23000E	00
0.20600E-01	0.40900E	00	0.28100E	01	0.28900E	00
0.13100E-01	0.48400E	00	0.10750E	01	0.94200E	00
0.18600E-01	0.35700E	00	0.15900E	01	0.15300E	00

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.97628E-04 PARAMETERS	SQRT(PHI)/ND= 0.82339E-03 0.17200E-01	0.59700E 00	LAMBDA= 0.10000E-01 0.46900E 00	-0.23500E 00
PHI= 0.86579E-04 PARAMETERS	SQRT(PHI)/ND= 0.77539E-03 0.17236E-01	0.59699E 00	LAMBDA= 0.99999E-02 0.44839E 00	-0.22139E 00
PHI= 0.77008E-04 PARAMETERS	SQRT(PHI)/ND= 0.73128E-03 0.17325E-01	0.59699E 00	LAMBDA= 0.99999E-02 0.39806E 00	-0.18552E 00
PHI= 0.74307E-04 PARAMETERS	SQRT(PHI)/ND= 0.71834E-03 0.17568E-01	0.56978E 00	LAMBDA= 0.99999E-03 0.38281E 00	-0.19386E 00
PHI= 0.74303E-04 PARAMETERS	SQRT(PHI)/ND= 0.71833E-03 0.17573E-01	0.56926E 00	LAMBDA= 0.99999E 02 0.38250E 00	-0.19403E 00
PHI= 0.74302E-04 PARAMETERS	SQRT(PHI)/ND= 0.71832E-03 0.17578E-01	0.56876E 00	LAMBDA= 0.99999E 02 0.38221E 00	-0.19421E 00
PHI= 0.70634E-04 PARAMETERS	SQRT(PHI)/ND= 0.70037E-03 0.18213E-01	0.56875E 00	LAMBDA= 0.99999E 00 0.36239E 00	-0.16803E 00

ALGORITHM TERMINATED

PHI= 0.70634E-04 PARAMETERS	SQRT(PHI)/ND= 0.70037E-03 0.18213E-01	0.56875E 00	LAMBDA= 0.10000E 04 0.36239E 00	-0.16803E 00
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SINGULAR MATRIX

DEPENDENT	DIFFERENCE	INDEPENDENT		2	3		
		1					
0.58500E-02	-0.23200E-02	0.48200E	00	0.10000E	00	0.50800E	00
0.26931E-01	-0.19310E-02	0.24590E	01	0.52700E	00	0.51500E	00
0.26930E-01	0.50696E-02	0.24500E	01	0.53000E	00	0.51500E	00
0.79175E-02	-0.23875E-02	0.47700E	00	0.49400E	00	0.25380E	00
0.11389E-01	-0.26891E-02	0.51400E	00	0.54000E	00	0.45500E	00
0.10878E-01	0.30410E-02	0.47300E	00	0.55200E	00	0.47300E	00
0.10882E-01	-0.12821E-02	0.47000E	00	0.55800E	00	0.47300E	00
0.46832E-02	0.45675E-03	0.10400E	00	0.56200E	00	0.44000E	00
0.21611E-01	-0.24118E-02	0.45000E	00	0.28400E	01	0.23000E	00
0.19622E-01	0.97726E-03	0.40900E	00	0.28100E	01	0.28900E	00
0.12499E-01	0.60047E-03	0.48400E	00	0.10750E	01	0.94200E	00
0.16442E-01	0.21578E-02	0.35700E	00	0.15900E	01	0.15300E	00

CORRELATION MATRIX

1.000			
-1.000	1.000		
-1.000	1.000	1.000	
-1.000	1.000	1.000	1.000

7 STEPS

DEPENDENT	INDEPENDENT		
	1	2	3
0.29800E-02	0.47800E 00	0.10200E 00	0.52500E C
0.38900E-01	0.25050E 01	0.51800E 00	0.49700E C
0.45000E-01	0.25000E 01	0.51700E 00	0.48500E C
0.20600E-01	0.42500E 00	0.27700E 01	0.31000E C
0.18500E-01	0.43300E 00	0.28000E 01	0.27000E C
0.18000E-01	0.48900E 00	0.56200E 00	0.51000E-C
0.10300E-01	0.54600E 00	0.50600E 00	0.44600E C
0.12150E-01	0.46900E 00	0.55600E 00	0.47500E C
C.7C500E-02	0.10000E 00	0.54000E 00	0.46400E C
0.82400E-02	0.42200E 00	0.46200E 00	0.26150E C
0.73400E-02	0.46700E 00	0.48500E 00	0.25550E C
C.31900E-01	0.14950E 01	0.51100E 00	0.49500E C
0.43500E-01	0.12220E 01	0.77600E 00	0.10300E C

MATRIX 1 IS A + SL*D
 MATRIX 2 IS A + SL*I
 MATRIX 3 IS A + SL*D-1

PHI= 0.29902E-03 PARAMETERS	SQRT(PHI)/ND= 0.13301E-02 0.23200E-01 0.70400E 00	LAMBDA= 0.10000E-01 0.48300E 00 -0.17900E 0
PHI= 0.21386E-03 PARAMETERS	SQRT(PHI)/ND= 0.11249E-02 0.26705E-01 0.71151E 00	LAMBDA= 0.99999E 00 0.28984E 00 -0.94066E-0
PHI= 0.20882E-03 PARAMETERS	SQRT(PHI)/ND= 0.11116E-02 0.26450E-01 0.73954E 00	LAMBDA= 0.99999E-01 0.29755E 00 -0.90030E-0
PHI= 0.20879E-03 PARAMETERS	SQRT(PHI)/ND= 0.11115E-02 0.26390E-01 0.74707E 00	LAMBDA= 0.99999E 01 0.29942E 00 -0.89086E-0
PHI= 0.20384E-03 PARAMETERS	SQRT(PHI)/ND= 0.10982E-02 0.24420E-01 0.74709E 00	LAMBDA= 0.99999E 00 0.30395E 00 -0.96450E-0
PHI= 0.20129E-03 PARAMETERS	SQRT(PHI)/ND= 0.10913E-02 0.24627E-01 0.71803E 00	LAMBDA= 0.99999E 00 0.29684E 00 -0.10007E 0
PHI= 0.20118E-03 PARAMETERS	SQRT(PHI)/ND= 0.10910E-02 0.24692E-01 0.71008E 00	LAMBDA= 0.99999E 01 0.29467E 00 -0.10121E 0
PHI= 0.19318E-03 PARAMETERS	SQRT(PHI)/ND= 0.10691E-02 0.25690E-01 0.71200E 00	LAMBDA= 0.99999E-01 0.29458E 00 -0.10033E 0
PHI= 0.19260E-03 PARAMETERS	SQRT(PHI)/ND= 0.10675E-02 0.25655E-01 0.71596E 00	LAMBDA= 0.99999E-02 0.29568E 00 -0.99754E-0
PHI= 0.19223E-03 PARAMETERS	SQRT(PHI)/ND= 0.10665E-02 0.25628E-01 0.71912E 00	LAMBDA= 0.99999E-02 0.29654E 00 -0.99296E-0
PHI= 0.19199E-03 PARAMETERS	SQRT(PHI)/ND= 0.10658E-02 0.25606E-01 0.72166E 00	LAMBDA= 0.99999E-02 0.29723E 00 -0.98933E-0
PHI= 0.19183E-03 PARAMETERS	SQRT(PHI)/ND= 0.10654E-02 0.25589E-01 0.72371E 00	LAMBDA= 0.99999E-02 0.29778E 00 -0.98644E-0
PHI= 0.19172E-03 PARAMETERS	SQRT(PHI)/ND= 0.10651E-02 0.25576E-01 0.72537E 00	LAMBDA= 0.99999E-02 0.29823E 00 -0.98411E-0
PHI= 0.19165E-03 PARAMETERS	SQRT(PHI)/ND= 0.10649E-02 0.25565E-01 0.72675E 00	LAMBDA= 0.99999E-03 0.29858E 00 -0.98223E-0
PHI= 0.19160E-03 PARAMETERS	SQRT(PHI)/ND= 0.10647E-02 0.25555E-01 0.72787E 00	LAMBDA= 0.99999E-03 0.29888E 00 -0.98069E-0
PHI= 0.19157E-03 PARAMETERS	SQRT(PHI)/ND= 0.10646E-02 0.25547E-01 0.72882E 00	LAMBDA= 0.99999E-04 0.29909E 00 -0.97945E-0
PHI= 0.19108E-03 PARAMETERS	SQRT(PHI)/ND= 0.10633E-02 0.25534E-01 0.73067E 00	LAMBDA= 0.99999E-05 0.29930E 00 -0.98116E-0
PHI= 0.19107E-03 PARAMETERS	SQRT(PHI)/ND= 0.10633E-02 0.25527E-01 0.73155E 00	LAMBDA= 0.99999E-03 0.29954E 00 -0.97995E-0
PHI= 0.19105E-03 PARAMETERS	SQRT(PHI)/ND= 0.10632E-02 0.25519E-01 0.73223E 00	LAMBDA= 0.99999E-04 0.29971E 00 -0.97916E-0
PHI= 0.19056E-03	SQRT(PHI)/ND= 0.10618E-02	LAMBDA= 0.99999E-05