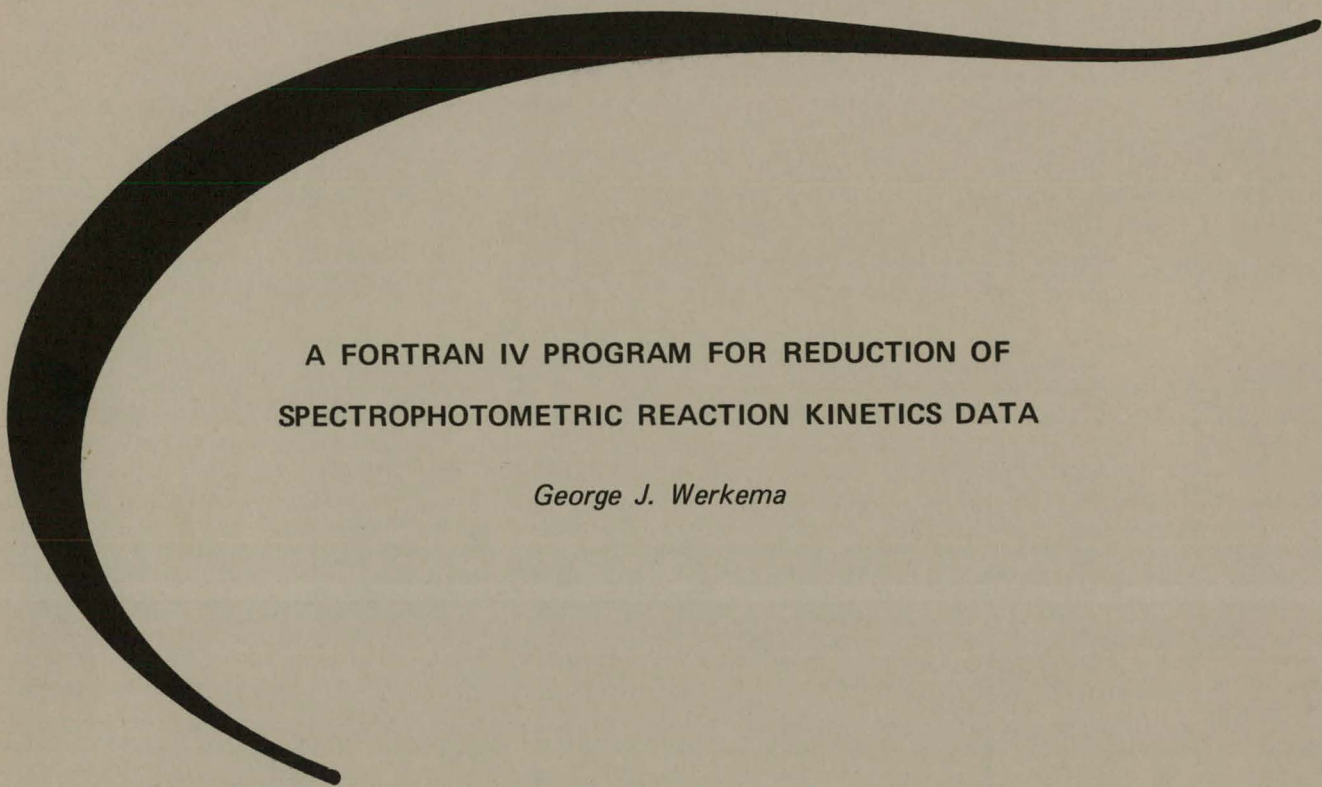


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MASTER



A FORTRAN IV PROGRAM FOR REDUCTION OF
SPECTROPHOTOMETRIC REACTION KINETICS DATA

George J. Werkema



THE DOW CHEMICAL COMPANY
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U.S. ATOMIC ENERGY COMMISSION
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CONTENTS

| | |
|---------------------------------------|---|
| Abstract | 1 |
| Introduction | 1 |
| Mathematical Methods | 1 |
| Reduction of Observational Data | 1 |
| Derivation of Integrated Laws | 3 |
| FORTTRAN Notation | 4 |
| Output | 5 |
| Input | 6 |
| Output | 7 |
| Program Listing | 9 |

A FORTRAN IV PROGRAM FOR REDUCTION OF SPECTROPHOTOMETRIC REACTION KINETICS DATA

George J. Werkema

Abstract. This program is a modification of one written earlier¹ for a small computer. The present version is written in E-level FORTRAN IV for the IBM 360-40G computer. The program reduces spectrophotometric absorbancy data to molar concentrations of reactants and products and, at the user's option, computes the rate constant time products ($k_1 t$, $k_2 t$, and $k_3 t$) using the integrated forms of first-, second-, and third-order rate laws.

INTRODUCTION

The reduction of spectrophotometric reaction kinetics data to molar concentrations of reactants and products is a tedious process. The ERLF program¹ and the present modification, ERLF-2, were written to perform the appropriate reduction and to test the reaction rate dependency. ERLF-2 is written in E-level FORTRAN IV for the IBM 360-40G computer.

The experiment for which ERLF-2 was written consists of observing the absorbance of visible or ultraviolet light at some discrete wavelength by one of the reaction constituents at several times during the course of a chemical reaction. Provision has been made in the program to correct for a minor interference from a chemical species whose concentration-rate-of-change is the negative of that for the species whose absorbance predominates at the observed wavelength. The mathematical derivation of the algorithm for these calculations is presented in the first paragraph of the next section.

The program has been written for chemical reactions of the type $A + B \rightleftharpoons C + D$. Species B and D are assumed to have zero absorbance at the observed wavelength. Species A and C have measurable absorbance at the observed wavelength with one species predominating by virtue of the relative magnitude of its molar extinction coefficient. That is, the molar extinction coefficient for species A at the observed wavelength must be much greater than that for species C if the observed data correspond to a decreasing concentration of species A. Conversely, if the

absorbancy increases during the course of the reaction, corresponding to an increase in the concentration of species C, then the molar extinction coefficient for species C at the observed wavelength must be much greater than that for species A. In general, these conditions are satisfied by standard spectrophotometric technique.

The program calculates the concentrations of species A, B, and C for each datum and then proceeds to compute the corresponding rate constant time products ($k_1 t$, $k_2 t$, and $k_3 t$) using the integrated forms of first-, second- and third-order rate laws. Division of the time products by the elapsed time at each datum gives a number whose constancy, or lack of, throughout a reaction is an indication of the order of the reaction. Values of this number are also listed for each datum. Derivations of these algorithms are presented in the second paragraph of the next section.

MATHEMATICAL METHODS

We define a general stoichiometry factor, P, such that the stoichiometric equation may be written

$$d[A] = p \cdot d[B] \quad (1)$$

This equation states that one gram-molecular-weight of B reacts stoichiometrically with P gram-molecular-weights of A. P need not be integral insofar as this program is concerned.

Reduction of Observational Data

In dilute solution, the absorbance of a species (A) in solution for a given wavelength of light (λ) is equal to the product of its molar extinction coefficient (ϵ_A^λ) and its concentration, [A], that is

$$(\text{Absorbance})_A^\lambda = \epsilon_A^\lambda [A]. \quad (2)$$

The total observed absorbance (Q^λ) of a solution at a given wavelength is equal to the sum of contributions due to all absorbing species and may be expressed as

$$Q^\lambda = \epsilon_A^\lambda [A] + \epsilon_B^\lambda [B] + \epsilon_C^\lambda [C] + \dots \quad (3)$$

¹ G. J. Werkema, "FORTRAN II Program for Reduction of Spectrophotometric Reaction Kinetics Data," RFP-629, Rocky Flats Division, The Dow Chemical Company, November 1965.

This program has been written to accommodate two absorbing species, one of which is a reactant, the other a product. In the ensuing discussion it is assumed that A is a reactant, C is a product, the contribution to the absorbance at λ_1 is due primarily to A and the contribution to the absorbance at λ_2 is due primarily to C. In addition, it is required that $-d[A] = d[C]$. The following paragraphs develop the relationships among these elements.

Absorbance at λ_1 : following the decrease of [A], with

$$\epsilon_A^{\lambda_1} > \epsilon_C^{\lambda_1}$$

The absorbance at λ_1 is equal to the sum of absorbances of the individual species present, that is, species A and C. Thus we have

$$Q^{\lambda_1} = \epsilon_A^{\lambda_1}[A] + \epsilon_C^{\lambda_1}[C], \quad (4)$$

with the contribution due to A being much larger. The amount of product C, [C], present is equal to the sum of the amount initially present plus that which was produced at the expense of A during the reaction, that is

$$[C] = [C]_0 + \{[A]_0 - [A]\} \quad (5)$$

Equation (5) is valid only if $-d[A] = d[C]$.

Substituting (5) in (4) gives

$$Q^{\lambda_1} = \epsilon_A^{\lambda_1}[A] + \epsilon_C^{\lambda_1}[C]_0 + \epsilon_C^{\lambda_1}\{[A]_0 - [A]\} \quad (6)$$

$$\text{Now let } \alpha^{\lambda_1} = Q^{\lambda_1} - \epsilon_C^{\lambda_1}[C]_0 \quad (7)$$

α^{λ_1} is, by this formulation, equal to the observed absorbance at λ_1 minus the absorbance due to any product C which was present at zero time. Upon substitution of (7), (6) becomes

$$\alpha^{\lambda_1} = \epsilon_A^{\lambda_1}[A] + \epsilon_C^{\lambda_1}[A]_0 - \epsilon_C^{\lambda_1}[A] \quad (8)$$

Rearranging (8) by solving for [A] gives

$$[A] = \frac{\alpha^{\lambda_1} - \epsilon_C^{\lambda_1}[A]_0}{\epsilon_A^{\lambda_1} - \epsilon_C^{\lambda_1}} \quad (9)$$

Equation (9) is the programmed formula. The concentration of reactant B, [B], is determined by the stoichiometric relationship of Equation (1). Note that in Equation (7) the correction to be applied must derive from some independent source. Usually, the most convenient way to do this

is to extrapolate the absorbance at λ_2 to zero time, which mainly is due to [C]. The ratio of the extinction coefficients for C at λ_1 and λ_2 is the scale factor necessary to compute the correction. That is,

$$\epsilon_C^{\lambda_1}[C]_0 = \frac{Q_{\text{initial}}^{\lambda_2} \cdot \epsilon_C^{\lambda_1}}{\epsilon_C^{\lambda_2}} \quad (10)$$

Absorbance at λ_2 : following the increase of [C], with

$$\epsilon_C^{\lambda_2} > \epsilon_A^{\lambda_2}$$

The absorbance at λ_2 is equal to the sum of absorbances of the individual species present, A and C. Using the formulation of Equation (4), we have the following expression:

$$Q^{\lambda_2} = \epsilon_A^{\lambda_2}[A] + \epsilon_C^{\lambda_2}[C]_T, \quad (11)$$

with the contribution due to C being much larger. $[C]_T$ is the total amount of product C present.

$$[C]_T = [C]_0 + [C], \quad (12a)$$

where [C] is the amount of product C which has been produced at the expense of A during the studied portion of the reaction, that is,

$$[C] = [A]_0 - [A] \quad (12b)$$

Let us rewrite (12b) to obtain

$$[A] = [A]_0 - [C] \quad (12c)$$

Upon substituting (12a) and (12c) in (11) we obtain

$$Q^{\lambda_2} = \epsilon_A^{\lambda_2}[A]_0 - \epsilon_A^{\lambda_2}[C] + \epsilon_C^{\lambda_2}[C]_0 + \epsilon_C^{\lambda_2}[C] \quad (13)$$

Now let

$$\alpha^{\lambda_2} = Q^{\lambda_2} - \epsilon_C^{\lambda_2}[C]_0 \quad (14)$$

Then

$$\alpha^{\lambda_2} = \epsilon_A^{\lambda_2}[A]_0 + (\epsilon_C^{\lambda_2} - \epsilon_A^{\lambda_2}) \cdot [C] \quad (15)$$

Rearranging (15) by solving for [C] gives

$$[C] = \frac{\alpha^{\lambda_2} - \epsilon_A^{\lambda_2}[A]_0}{\epsilon_C^{\lambda_2} - \epsilon_A^{\lambda_2}} \quad (16)$$

Equation (16) is the programmed formula and is in the same form as Equation (9). Note that all dependence on the variability of [A] has been removed. The quantity $\epsilon_C^{\lambda^2}[C]_0$ is the measured or extrapolated absorbancy due to the species C at zero time, which is, exactly

$\alpha_{\text{initial}}^{\lambda^2} \epsilon_A^{\lambda^2} [A]_0$, barring other interferences, the program determines whether to use Equation (9) or Equation (16) by comparing the relative magnitudes of $\epsilon_A^{\lambda^2}$ and $\epsilon_C^{\lambda^2}$. If $\epsilon_A^{\lambda^2} > \epsilon_C^{\lambda^2}$, Equation (9) is used; otherwise, the program chooses Equation (16). The condition $\epsilon_A^{\lambda^2} = \epsilon_C^{\lambda^2}$ is regarded as an error and the job is terminated.

Derivation of Integrated Rate Laws

First-Order Rate Law: The subprogram has been written for the special case in which the reaction rate is first-order in reactant B, that is

$$\frac{-d[A]}{dt} = k_1 \cdot [B]$$

in which k_1 is the first-order rate constant. The integrated form of this first-order rate equation is:

$$k_1 t = P \cdot \ln\left(\frac{[B]_0}{[B]}\right),$$

where [B] = concentration of component B at any time in moles/liter, $[B]_0$ = initial concentration of component B in moles/liter and P = stoichiometry factor.

Second-Order Rate Law: The subprogram has been written for the special case in which the reaction is first-order in each reactant A and B, that is

$$\frac{-d[A]}{dt} = k_2 [A] \cdot [B],$$

in which k_2 is the second-order rate constant. The integrated form of this second-order rate equation is

$$k_2 t = \frac{P}{P \cdot [B]_0 \cdot [A]_0} \ln \frac{[A]_0 \cdot [B]}{[B]_0 \cdot [A]},$$

where [A] = concentration of component A at any time, in moles/liter, $[A]_0$ = initial concentration of component A, in moles/liter and similarly for [B] and $[B]_0$.

Third-Order Rate Law: The subprogram has been written for the special case in which the reaction rate is second-order in component A and first-order in component B, that is

$$\frac{-d[A]}{dt} = k_3 [A]^2 \cdot [B],$$

in which k_3 is the third-order rate constant. The integrated form of this third-order rate equation is

$$k_3 t = \frac{P}{P \cdot [B]_0 \cdot [A]_0} \left(\frac{1}{[A]} - \frac{1}{[A]_0} \right) + \frac{P}{(P \cdot [B]_0 \cdot [A]_0)^2} \ln \frac{[B]_0 [A]}{[A]_0 [B]},$$

With the symbolic significances as before.

The program user may select any or all of the integrated rate law calculation routines. At least one must be specified in order to obtain printed output. The routines are selected by means of three control characters, L1, L2, and L3, whose control functions are tabulated as follows:

If L1: = 0, do not calculate first-order rate constant; go on to test L2;

> 0, compute and output reduced data and first order rate constants, then test L2.

If L2: = 0, do not calculate second-order rate constants; go on to test L3;

> 0, compute and output reduced data and second-order rate constants, then test L3.

If L3: = 0, do not calculate third-order rate constants; go on to termination routine;

> 0, compute and output reduced data and third-order rate constants, then go to termination routine.

FORTRAN NOTATION

The mathematical symbols used in the previous discussion are represented in the FORTRAN source program by the labels indicated as follows:

| <u>Mathematical Symbol</u> | <u>FORTRAN Label</u> | <u>Mathematical Symbol</u> | <u>FORTRAN Label</u> |
|----------------------------|----------------------|----------------------------|----------------------|
| $[A]_0$ | AO | $\alpha \lambda_n$ | ABNS(I) |
| $[B]_0$ | BO | $\epsilon \lambda_n$ | BRACK |
| $[C]_0$ | CO | t | X(I) |
| [A] | Y(I) | k_1 | C1 |
| [B] | BT(I) | k_2 | C2 |
| [C] | CT(I) | k_3 | C3 |
| P | P | $k_1 t$ | C1T |
| $\epsilon_A^{\lambda_n}$ | E3 | $k_2 t$ | C2T |
| $\epsilon_C^{\lambda_n}$ | E4 | $k_3 t$ | C3T |
| | | L1, L2, L3 | L1, L2, L3 |

INPUT

| <u>Card</u> | <u>Column</u> | <u>Format</u> | <u>Label</u> | <u>Description</u> | <u>Card</u> | <u>Column</u> | <u>Format</u> | <u>Label</u> | <u>Description</u> |
|-------------|---------------|---------------|--------------|---|-------------|---------------|---------------|--------------|---|
| | 5-8 | I4 | NJOB | Number of experimental data sets to be processed sequentially | | 21-28 | F8.6 | BO | Initial concentration of species B |
| 2 | 5-8 | I4 | NRUN | Run number, for experiment identification | | 29-36 | F8.6 | CO | Initial concentration of species C |
| | 9-12 | I4 | NDP | Number of data points recorded in the experiment | | 37-44 | F8.6 | P | Stoichiometry factor (d[A] = Pd[B]) |
| | 13-80 | 17A4 | TITLE | Alphanumeric information | | 45-52 | F8.3 | E3 | Molar extinction coefficient of species A |
| 3 | 10 | I1 | L1 | First-order control character | | 53-60 | F8.3 | E4 | Molar extinction coefficient of species C |
| | 11 | I1 | L2 | Second-order control character | | | | | |
| | 12 | I1 | L3 | Third-order control character | 4 | 13-20 | F8.2 | X(I) | Time |
| | 13-20 | F8.6 | AO | Initial concentration of species A | | 21-28 | F8.3 | ABNS(I) | Absorbance |

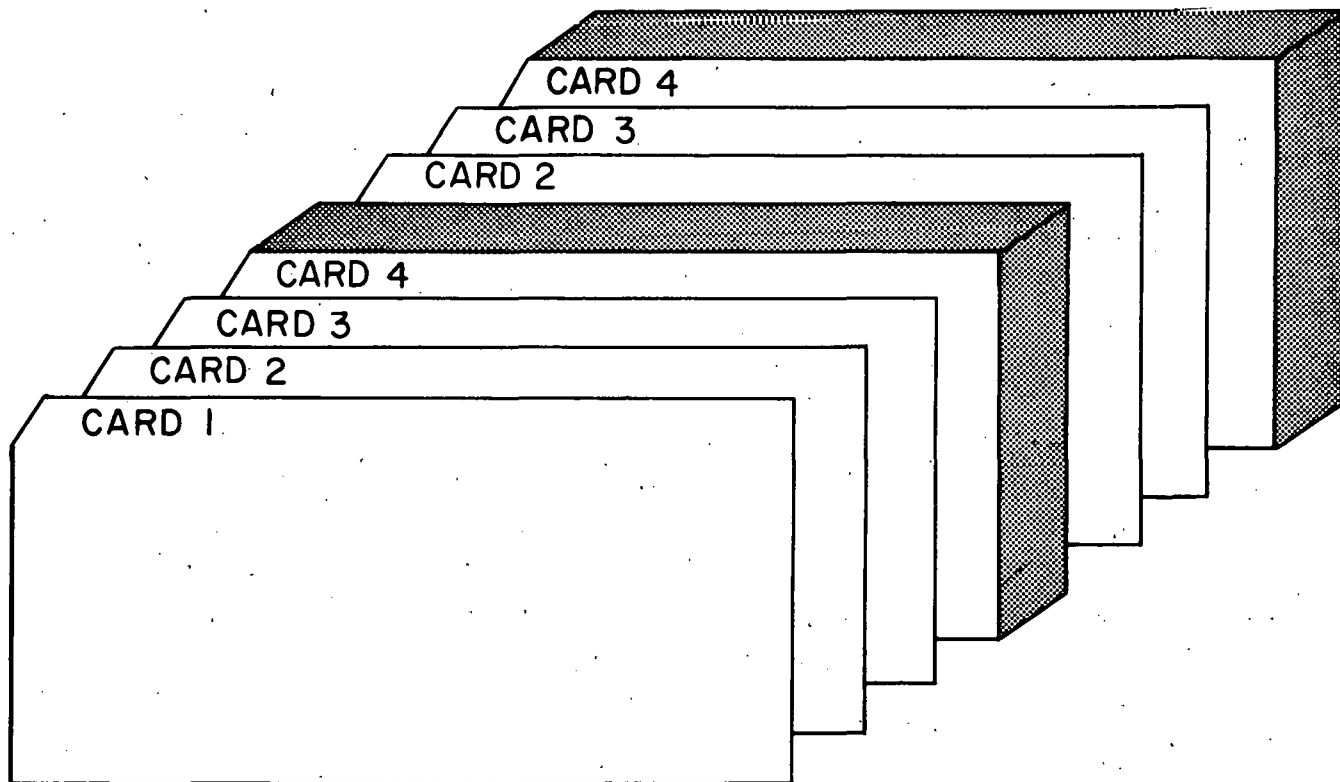


Figure 1. Data Deck.

Prepare one card 1 for each computer job. One each of cards 2 and 3 are needed for each experimental run. Card 4 is a data point card and one is needed for each absorbance reading. Figure 1 shows a schematic of a deck make-up for a computer job which will process absorbance readings from two experimental runs.

OUTPUT

For each of the integrated reaction rate law calculations that is selected, one table is listed on the printer. The tables are arranged with the following format: line 1 is the "TITLE," reproduced verbatim from the information on data card 2; line 2 is self-explanatory and contains the input constants NRUN, AO, BO, and CO; the column headings for the result table are, left to right, T, X, A, B, C, K l , K l /T. T is time; X is the number of gram-molecular-weights of species B reacted ($=[B]_0 - [B]$); A, B, and C are the numbers of gram-molecular-weights of species A, B, and C respectively, present in the reaction mixture; K l , where $l = 1, 2, \text{ or } 3$ depending on the order of the integrated law calculation, is the computed rate constant time product divided by the time datum; K l /T, with l as defined before, is the computed rate constant time product. These results are computed for each absorbance measurement.

SAMPLE OUTPUT

NPV-XE03 1M HCL04 60C

RUN NO. 941 A0 = 0.021227 B0 = 0.007930 C0 = 0.000646

| T | X | A | B | C | K2 | K2T |
|---------|----------|----------|----------|----------|----------|------------|
| 13.00 | 0.000020 | 0.021105 | 0.007910 | 0.000768 | 0.055964 | 0.727527 |
| 52.00 | 0.000062 | 0.020853 | 0.007868 | 0.001020 | 0.036346 | 2.253483 |
| 259.00 | 0.000256 | 0.019691 | 0.007674 | 0.002182 | 0.037184 | 9.630732 |
| 380.00 | 0.000340 | 0.019186 | 0.007590 | 0.002687 | 0.034304 | 13.035463 |
| 607.00 | 0.000466 | 0.018428 | 0.007464 | 0.003445 | 0.030294 | 18.388367 |
| 731.00 | 0.000542 | 0.017974 | 0.007388 | 0.003899 | 0.029756 | 21.751816 |
| 1341.00 | 0.000795 | 0.016459 | 0.007135 | 0.005414 | 0.025267 | 33.883621 |
| 1560.00 | 0.000854 | 0.016105 | 0.007076 | 0.005768 | 0.023679 | 36.939621 |
| 1808.00 | 0.000913 | 0.015751 | 0.007017 | 0.006122 | 0.022173 | 40.089523 |
| 2776.00 | 0.001174 | 0.014186 | 0.006756 | 0.007687 | 0.019920 | 55.297745 |
| 3230.00 | 0.001266 | 0.013630 | 0.006664 | 0.008243 | 0.018963 | 61.251801 |
| 4561.00 | 0.001527 | 0.012065 | 0.006403 | 0.009808 | 0.017526 | 79.937775 |
| 5872.00 | 0.001738 | 0.010802 | 0.006192 | 0.011071 | 0.016604 | 97.498169 |
| 7114.00 | 0.001914 | 0.009741 | 0.006016 | 0.012132 | 0.016086 | 114.434326 |
| 7590.00 | 0.001973 | 0.009388 | 0.005957 | 0.012485 | 0.015891 | 120.609833 |

NPV-XE03 1M HCL04 60C

RUN NO. 941 A0 = 0.021227 B0 = 0.007930 C0 = 0.000646

| T | X | A | B | C | K3 | K3T |
|---------|----------|----------|----------|----------|----------|-------------|
| 13.00 | 0.000020 | 0.021105 | 0.007910 | 0.000768 | 2.644715 | 34.381302 |
| 52.00 | 0.000062 | 0.020853 | 0.007868 | 0.001020 | 1.727763 | 107.121353 |
| 259.00 | 0.000256 | 0.019691 | 0.007674 | 0.002182 | 1.819657 | 471.291260 |
| 380.00 | 0.000340 | 0.019186 | 0.007590 | 0.002687 | 1.701234 | 646.468994 |
| 607.00 | 0.000466 | 0.018428 | 0.007464 | 0.003445 | 1.534090 | 931.193115 |
| 731.00 | 0.000542 | 0.017974 | 0.007388 | 0.003899 | 1.526687 | 1116.008301 |
| 1341.00 | 0.000795 | 0.016459 | 0.007135 | 0.005414 | 1.358525 | 1821.783203 |
| 1560.00 | 0.000854 | 0.016105 | 0.007076 | 0.005768 | 1.288133 | 2009.487305 |
| 1808.00 | 0.000913 | 0.015751 | 0.007017 | 0.006122 | 1.220830 | 2207.260986 |
| 2776.00 | 0.001174 | 0.014186 | 0.006756 | 0.007687 | 1.161908 | 3225.457031 |
| 3230.00 | 0.001266 | 0.013630 | 0.006664 | 0.008243 | 1.131174 | 3653.694580 |
| 4561.00 | 0.001527 | 0.012065 | 0.006403 | 0.009808 | 1.120879 | 5112.332031 |
| 5872.00 | 0.001738 | 0.010802 | 0.006192 | 0.011071 | 1.132806 | 6651.835937 |
| 7114.00 | 0.001914 | 0.009741 | 0.006016 | 0.012132 | 1.167276 | 8304.007812 |
| 7590.00 | 0.001973 | 0.009388 | 0.005957 | 0.012485 | 1.179163 | 8949.847656 |

SAMPLE OUTPUT (Continued)

NPV-XE03 1M HCL04 60C

RUN NO. 942 AO = 0.021364 BO = 0.007930 CO = 0.000636

| T | X | A | B | C | K2 | K2T |
|---------|----------|----------|----------|----------|----------|------------|
| 8.00 | 0.000012 | 0.021293 | 0.007918 | 0.000707 | 0.052526 | 0.420211 |
| 63.00 | 0.000062 | 0.020990 | 0.007868 | 0.001010 | 0.035497 | 2.236298 |
| 253.00 | 0.000239 | 0.019929 | 0.007691 | 0.002071 | 0.035188 | 8.902465 |
| 381.00 | 0.000357 | 0.019222 | 0.007573 | 0.002778 | 0.035790 | 13.635991 |
| 609.00 | 0.000475 | 0.018515 | 0.007455 | 0.003485 | 0.030582 | 18.624161 |
| 731.00 | 0.000559 | 0.018010 | 0.007371 | 0.003990 | 0.030581 | 22.354950 |
| 1342.00 | 0.000820 | 0.016444 | 0.007110 | 0.005556 | 0.026021 | 34.920303 |
| 1561.00 | 0.000879 | 0.016091 | 0.007051 | 0.005909 | 0.024337 | 37.989716 |
| 1810.00 | 0.000938 | 0.015737 | 0.006992 | 0.006263 | 0.022737 | 41.153641 |
| 2777.00 | 0.001190 | 0.014222 | 0.006740 | 0.007778 | 0.020131 | 55.904068 |
| 3231.00 | 0.001283 | 0.013667 | 0.006647 | 0.008333 | 0.019145 | 61.857574 |
| 4562.00 | 0.001510 | 0.012303 | 0.006420 | 0.009697 | 0.017087 | 77.952606 |
| 5874.00 | 0.001687 | 0.011242 | 0.006243 | 0.010758 | 0.015695 | 92.195145 |
| 7115.00 | 0.001838 | 0.010333 | 0.006092 | 0.011667 | 0.014880 | 105.870117 |
| 7591.00 | 0.001864 | 0.010182 | 0.006066 | 0.011818 | 0.014267 | 108.300003 |

NPV-XE03 1M HCL04 60C

RUN NO. 942 AO = 0.021364 BO = 0.007930 CO = 0.000636

| T | X | A | B | C | K3 | K3T |
|---------|----------|----------|----------|----------|----------|-------------|
| 8.00 | 0.000012 | 0.021293 | 0.007918 | 0.000707 | 2.465637 | 19.725098 |
| 63.00 | 0.000062 | 0.020990 | 0.007868 | 0.001010 | 1.676618 | 105.626923 |
| 253.00 | 0.000239 | 0.019929 | 0.007691 | 0.002071 | 1.706031 | 431.625977 |
| 381.00 | 0.000357 | 0.019222 | 0.007573 | 0.002778 | 1.767708 | 673.496826 |
| 609.00 | 0.000475 | 0.018515 | 0.007455 | 0.003485 | 1.540086 | 937.912354 |
| 731.00 | 0.000559 | 0.018010 | 0.007371 | 0.003990 | 1.562575 | 1142.243164 |
| 1342.00 | 0.000820 | 0.016444 | 0.007110 | 0.005556 | 1.395551 | 1872.829102 |
| 1561.00 | 0.000879 | 0.016091 | 0.007051 | 0.005909 | 1.320648 | 2061.532715 |
| 1810.00 | 0.000938 | 0.015737 | 0.006992 | 0.006263 | 1.248824 | 2260.373291 |
| 2777.00 | 0.001190 | 0.014222 | 0.006740 | 0.007778 | 1.169263 | 3247.043945 |
| 3231.00 | 0.001283 | 0.013667 | 0.006647 | 0.008333 | 1.137143 | 3674.109863 |
| 4562.00 | 0.001510 | 0.012303 | 0.006420 | 0.009697 | 1.077662 | 4916.292969 |
| 5874.00 | 0.001687 | 0.011242 | 0.006243 | 0.010758 | 1.043238 | 6127.980469 |
| 7115.00 | 0.001838 | 0.010333 | 0.006092 | 0.011667 | 1.039681 | 7397.335937 |
| 7591.00 | 0.001864 | 0.010182 | 0.006066 | 0.011818 | 1.005696 | 7634.242187 |

PROGRAM LISTING

```

C   ERLF  060666
      DIMENSION Y(60),ABNS(60),BR(60),X(60),BT(60),CT(60),TITLE(17)
      INPT = 1
      LIST = 3
      READ (INPT,2009)NJOB
2009  FORMAT(4X,I4)
      DO 82 JOB = 1,NJOB
41    READ(INPT,2010)NRUN,NDP,TITLE
2010  FORMAT(4X,2I4,17A4)
      READ(INPT,2011)L1,L2,L3,A0,B0,CO,P,E3,E4
2011  FORMAT(9X,3I1,4F8.6,2F8.3)
      A1 = P*B0-A0
      A2 = P/A1
      A3 = A2/A1
      A4 = A0/B0
      A5 = 1.0/A0
      A6 = E3*A0
      A7 = E4*A0
      A8 = 1.0/(P*(E4-E3))
      A9 = A0/P
      IF(E3-E4)141,82,241
141   LAM = 2
      GO TO 42
241   LAM = 1
42    DO 46 I = 1,NDP
      READ(INPT,2012)X(I),ABNS(I)
2012  FORMAT(12X,F8.2,F8.3)
      BRACK = ABNS(I)-CO*E4
      GO TO (44,45),LAM
44    BR(I) = A9 + (BRACK - A7)*A8
      GO TO 145
45    BR(I) = (BRACK - A6)*A8
145   Y(I) = A0 - P*BR(I)
      BT(I) = B0-BR(I)
46    CT(I) = CO + P*BR(I)
      IF(L1)82,48,47
47    WRITE(LIST,2020)TITLE
2020  FORMAT(4H1      ,17A4)
      WRITE(LIST,2021)NRUN,A0,B0,CO
2021  FORMAT(12HO  RUN NO. ,14,7H  A0 = ,F8.6,7H  B0 = ,F8.6,7H  CO = ,
1F8.6)
      WRITE(LIST,2022)
2022  FORMAT(77HO  T      X      A      B      C
1     K1      K1T)
      DO 147 I = 1,NDP
      C1T = P*ALOG(B0/BT(I))
      C1 = C1T/X(I)
147   WRITE(LIST,2023)X(I),BR(I),Y(I),BT(I),CT(I),C1,C1T

```

PROGRAM LISTING (Continued)

```

2023  FORMAT(1X,F8.2,6F12.6)
48    IF(L2)82,50,49
49    WRITE(LIST,2020)TITLE
      WRITE(LIST,2021)NRUN,A0,B0,CO
      WRITE(LIST,2024)
2024  FORMAT(77HO      T          X          A          B          C
1      K2          K2T)
      DO 149 I = 1,NDP
      C2T = A2*ALOG((A0*BT(I))/(B0*Y(I)))
      C2 = C2T/X(I)
149   WRITE(LIST,2023)X(I),BR(I),Y(I),BT(I),CT(I),C2,C2T
50    IF(L3)82,82,51
51    WRITE(LIST,2020)TITLE
      WRITE(LIST,2021)NRUN,A0,B0,CO
      WRITE(LIST,2025)
2025  FORMAT(77HO      T          X          A          B          C
1      K3          K3T)
      DO 151 I = 1,NDP
      FIR = ALOG((A0*BT(I))/(B0*Y(I)))
      C3T = A2/(Y(I)) - A2*A5 - A3*FIR
      C3 = C3T / X(I)
151   WRITE(LIST,2023)X(I),BR(I),Y(I),BT(I),CT(I),C3,C3T
82    CONTINUE
      CALL EXIT
      STOP
      END

```