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A nomograph for the rapid solution of the Arrhenius equation

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A NOMOGRAPH FOR THE RAPID SOLUTION OF THE ARRHENIUS EQUATION

BY

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ABSTRACT

There are presently no calculational aids for the rapid computation of the Arrhenius parameters of the chemical reaction rate equations.

Two nomographs for solving the Arrhenius equation for the relative reaction rate constants at different temperatures, and for computing activation energies and frequency factors are presented. Several graphs and tables of the relative reaction rate constant as a function of activation energy and temperature are also presented.

The nomographs, graphs and tables can be used, singly or combined, in lieu of numerical calculation for the solution for Arrhenius parameters, or the computation of rate constants.

A computer program included in the paper may be modified to obtain many more sets of data than are presented here.

APPROVAL OF THESIS

A NOMOGRAPH FOR THE RAPID SOLUTION

OF THE ARRHENIUS EQUATION

BY

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FOR

DEPARTMENT OF CHEMICAL ENGINEERING

NEWARK COLLEGE OF ENGINEERING

BY

FACULTY COMMITTEE

APPROVED: ______________________________

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PREFACE

The writer has attempted in this paper to present various calculational aids for computing the Arrhenius parameters of the reaction rate equation.

The nomographs, graphs, tables and programs in this paper may be used, singly or together, to obtain readily the required parameters for design or experimental work.

ACKNOWLEDGMENTS

I wish to express my sincerest thanks to Dr. S. I. Kreps for his help in preparing this paper. I wish to thank him and Dr. D. Hanesian for allowing me to read and use material from the manuscript of their forthcoming text on kinetics. I also wish to thank Dr. Kreps for the concept of using the G factor which he developed.

I would also like to take this opportunity to thank American Cyanamid Company for the use of the computer and the staff for their help in this paper. Some reduction work had to be done on the tables and graphs and I would like to thank the Graphic Services Department of Cyanamid for providing this service.

I would also like to thank Miss D. De Maio who proofread and typed this paper.

Last of all I would like to thank my wife and children for their help and support these thirteen years I have spent attaining an education in the evenings.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

Table		Page
21	Tabulated Values of k_2/k_1, T_1 = 900°C . . .	76
22	Tabulated Values of k_2/k_1, T_1 = 950°C . . .	77
23	Tabulated Values of k_2/k_1, T_1 =1000°C . . .	78
24	Values of (1-G)/G, ΔT = 10-100°C.	39
25	Values of (1-G)/G, ΔT = 1-10°C.	41

LIST OF COMPUTER PROGRAMS

INTRODUCTION

Rate Equation Defined

The rate of reaction of a reaction component can be defined as the moles of the component which appear by reaction in a unit volume and a unit time.[1] By convention if the component appears as a product, the rate of reaction is a positive quantity and if the component is disappearing, or is a reactant, the reaction rate is negative.

The variables which effect the rate of reaction are: 1. concentration of the components of the reaction, 2. the pressure at which the reaction occurs and 3. the temperature at which reaction occurs. Therefore, the reaction rate of a component is a function of temperature, pressure and concentration. The above three variables are dependent on one another and at equilibrium and at a given pressure, the reaction rate is dependent on temperature and concentration. The reaction rate, therefore, is expressed as a function of temperature and concentration. The form of the defining equation is

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[1] Octave Levenspiel, Chemical Reaction Engineering, John Wiley & Sons, Inc., New York, 1962, Chapter 2.

expressed as:

$$r_A = k\ (A)^N \qquad (1\text{-}1)$$

where

r_A = Reaction Rate, (concentration)(time)$^{-1}$

(A)= Concentration of Component A

k = Reaction Rate Constant, (time)$^{-1}$(concentration)$^{1-N}$

N = Exponent (order of reaction).

The above expression can be complex depending on the number of components involved.

Considering the reaction:

$$H_2 + Br_2 \longrightarrow 2HBr$$

the experimental rate equation for the formation of HBr is:

$$r_{HBr} = \frac{k_1\ (H_2)(Br_2)^{1/2}}{k_2 + (HBr)/(Br_2)} \qquad (1\text{-}2)$$

therefore, the expression for the rate equation is divided into two types of variables, concentration dependent terms and a time-concentration constant. The time-concentration constant or reaction rate constant is a function of temperature and is the subject of this paper.

The temperature dependent term must be expressed as a function of temperature. Svante August Arrhenius in 1889 developed an empirical relationship for the rate constant which is:

$$k = ko \exp(-E/RT) \quad (1\text{-}3)$$

where

ko = Frequency factor

E = Activation Energy, calories per gram mole

T = Absolute Temperature, degrees Kelvin

R = Ideal Gas Constant, 1.98719 calories per degree C, mole

The term ko above can also be expressed as a function of temperature and is:

$$ko = AT^{j} \qquad 0. \geq j \geq 1.0. \quad (1\text{-}4)$$

The reason for the variable power arises from the theoretical approach used to determine the temperature dependency of the rate constant. The two generally accepted theories are the Kinetic Collision Theory whose power, j, is one-half, and the Absolute Reaction Rate Theory, which uses a power of one. Kreps and Hanesian(2) have examined the above two theorems in relation to the Arrhenius method, which neglects the temperature dependent term in ko, and they have shown for a reaction, for example, at 540°K, the absolute rate theory corresponds within 5% over a 65°C range and the collision theory corresponds within 5% over a 35°C range. This paper does

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(2) Personal communication, Dr. S. I. Kreps, Professor of Chemical Engineering, Newark College of Engineering, January, 1971.

not attempt to study the various methods or theories but simply intends to provide a computational method for calculating the Arrhenius parameters.

Problem Defined

The Arrhenius equation has become the equation most often used to determine rate equations and activation energies. The equation as presented is:

$$k = ko \exp(-E/RT) \tag{1-3}$$

or

$$k = ko \times 10^{(-E/2.303RT)} \tag{1-3a}$$

The general application of this equation is to obtain two sets of experimental reaction rate data; one at some reference temperature T_1 and one at another temperature T_2, higher than T_1. Writing the reaction rate equation:

$$r_1 = k_{1(T_1)} \; C_A^N \tag{1-5}$$

and

$$r_2 = k_{2(T_2)} \; C_A^N \tag{1-4a}$$,

the rate constants $k_i(T_i)$ can be computed. The reaction rate constant equation (1-3) may be written in logarithmic form for both temperatures and becomes:

$$\ln k_1 = \ln ko - (E/RT_1) \tag{1-6}$$

$$\ln k_2 = \ln ko - (E/RT_2) \tag{1-7}$$

Subtracting (1-6) from (1-7) we obtain:

$$\ln k_2 - \ln k_1 = -(E/RT_2) + (E/RT_1) \qquad (1\text{-}8)$$

or

$$\ln (k_2/k_1) = -(E/R)(1/T_2 - 1/T_1) \qquad (1\text{-}8a)$$

or

$$\ln (k_2/k_1) = - E/R\ (T_1 - T_2/T_1 T_2) \qquad (1\text{-}8b)$$

The above equation (1-8b) is the one most widely used to calculate the Arrhenius parameter E and relative reaction rate constants. Knowing both temperatures and the reaction rate constants, it is a simple procedure to calculate the activation energy E. Also knowing the activation energy and the reaction rate at one temperature, the reaction rate at any other temperature is readily calculated. There are presently no calculational aids to the solution of these equations. This paper attempts to provide a nomograph which will decrease time spent in calculation and also to provide a series of graphs and tables of relative reaction rate constants as a function of activation energy and temperature.

DEVELOPMENT OF NOMOGRAPH

Computer Tables

Before the nomograph could be made it was necessary to determine the limits of the parameters involved so as to obtain a more meaningful nomograph. It was arbitrarily decided to keep the reference temperature between -100°C and 1,000°C and to hold ΔT to a maximum of 100°C. Activation energies were chosen to lie between 5,000 and 65,000 calories per gram mole which covers the range of most chemical reaction activations.

A computer program was written (Appendix) to permit machine computation of data points which were used to construct the nomograph. Tables were also generated for reference temperatures in increments of 50°C. and activation energies in increments of 5,000 calories per gram mole. Since the tabular values of k_2/k_1 were readily obtainable from the computer these data have been incorporated in this paper and can be used to the extent that the values presented be used as is, with no simple interpolation. Since the function tabulated is a logarithmic function the logarithms of these values would be needed to interpolate directly in the tables.

In obtaining the tables it was evident that some conditions where the temperature was low (-100°C to 200°C) and the activation energy was high (50,000 to 65,000 calories per gram mole) the k_2/k_1 values obtained were very high and were not considered useful for the nomograph. The program was then constructed so that k_2/k_1 values greater than 999 would not be printed.

Graphs

Having obtained the tabulated values via the computer program a set of graphs were constructed to permit the reader as much versatility as possible in choosing a method to rapidly determine the Arrhenius parameters, E and ko. Interpolation, again, is neither simple nor convenient between graphs, but all values of the activation energy may be used, and less error will develop on interpolation for the temperature difference than occurs when using the tables since by using a logarithmic scale for k_2/k_1 the logarithms are plotted and not the value of k_2/k_1.

Nomograph

Having obtained the necessary data, a form for the nomograph was needed. The equation to be considered was:

$$k = ko \exp - E/RT \qquad (2\text{-}1)$$

Using two experimental points and subtracting the equations (as developed earlier) the expression:

$$\ln (k_2/k_1) = - E/R\ (1/T_2 - 1/T_1) \qquad (2\text{-}2)$$

is obtained where:

$$T_2 > T_1.$$

If a factor G is introduced such that $T_2 = GT_1$ a substitution may be made and equation (2-2) may be written as:

$$\ln (k_2/k_1) = - E/R\ (1/GT_1 - 1/T_1) \qquad (2\text{-}2a)$$

Further manipulation by combining the two temperature terms and factoring results in:

$$\ln (k_2/k_1) = - E/R((1-G)/G)(1/T_1). \qquad (2\text{-}2b)$$

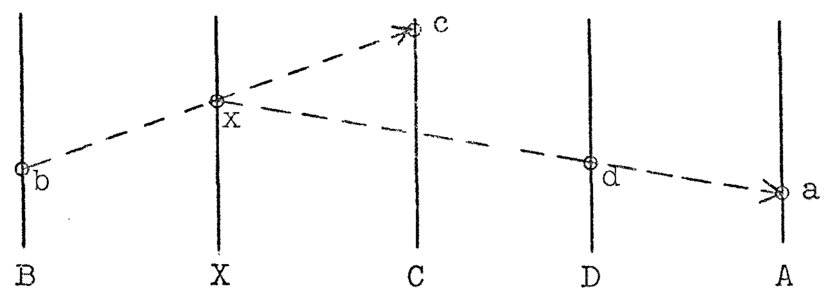
By using the factor G, the above equation simplifies to the form of:

$$\ln A = B \times C \times D \qquad (2\text{-}3)$$

which can readily be used to make a linear nomograph. The logarithm of the above equation can be obtained and the result can be expressed as:

$$\log (\log A) = \log (B/2.303) + \log C + \log D \qquad (2\text{-}4)$$

Equation (2-4) can be readily made into a nomograph consisting of parallel vertical lines in the form:

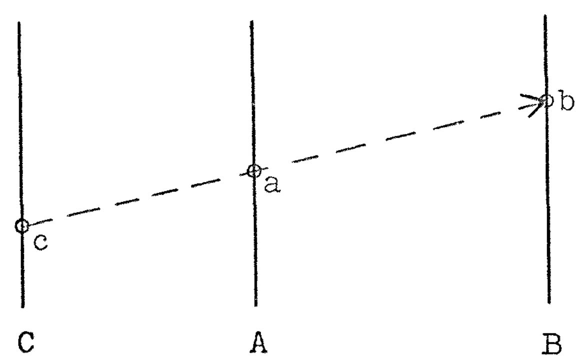


where X is a pivotal point equal to B x C.

A normal three variable equation can be written as:

$$\log A = \log B + \log C \qquad (2\text{-}5)$$

and the nomograph appears as:



where A is a linear function of B and C.

When there are more than three variables the equation must be broken into sets of three-variable equations, for example:

$$\log A = \log B + \log C + \log D \qquad (2\text{-}6)$$

the above may also be written as:

$$\log A - \log D = \log B + \log C = \log X \qquad (2\text{-}7)$$

The pivotal variable X is introduced and two sets of equations are available, that is:

$$\log A - \log D = \log X \tag{2-8}$$

and

$$\log B + \log C = \log X \tag{2-9}$$

We may then put two three-variable nomographs together to solve the problem.

Since there was no convenient way to express the value (1-G)/G it was convenient to make an additional nomograph to compute the value (1-G)/G which could then be used in the nomograph for k_2/k_1. The equation:

$$T_2 = G\ T_1 \tag{2-10}$$

was substituted into the expression:

$$(1-G)/G \tag{2-11}$$

which reduced to:

$$\frac{\Delta T}{T_2} = (1-G)/G \tag{2-12}$$

this is in the form of a three variable nomograph and is presented on Page 12. The nomograph is used by connecting a straight line between the value of T_2 and that of Δt and reading (1-G)/G on the middle scale. There is a low scale for Δt equal to 1-10°C, and a high scale for Δt equal to 10-100°C. For convenience, the G- function is also evaluated in tables and graphs in the appendix.

The main nomograph for obtaining k_2/k_1 was readily constructed using the two three-variable equations:

$$\frac{1}{T_1} \times \frac{E}{2.303R} = X \qquad (2\text{-}13)$$

and

$$X \times \frac{(1-G)}{G} = \log k_2/k_1. \qquad (2\text{-}14)$$

Printed logarithmic scales supplied in Burrows[3] were used to construct the scales. The nomograph is presented on Page 13.

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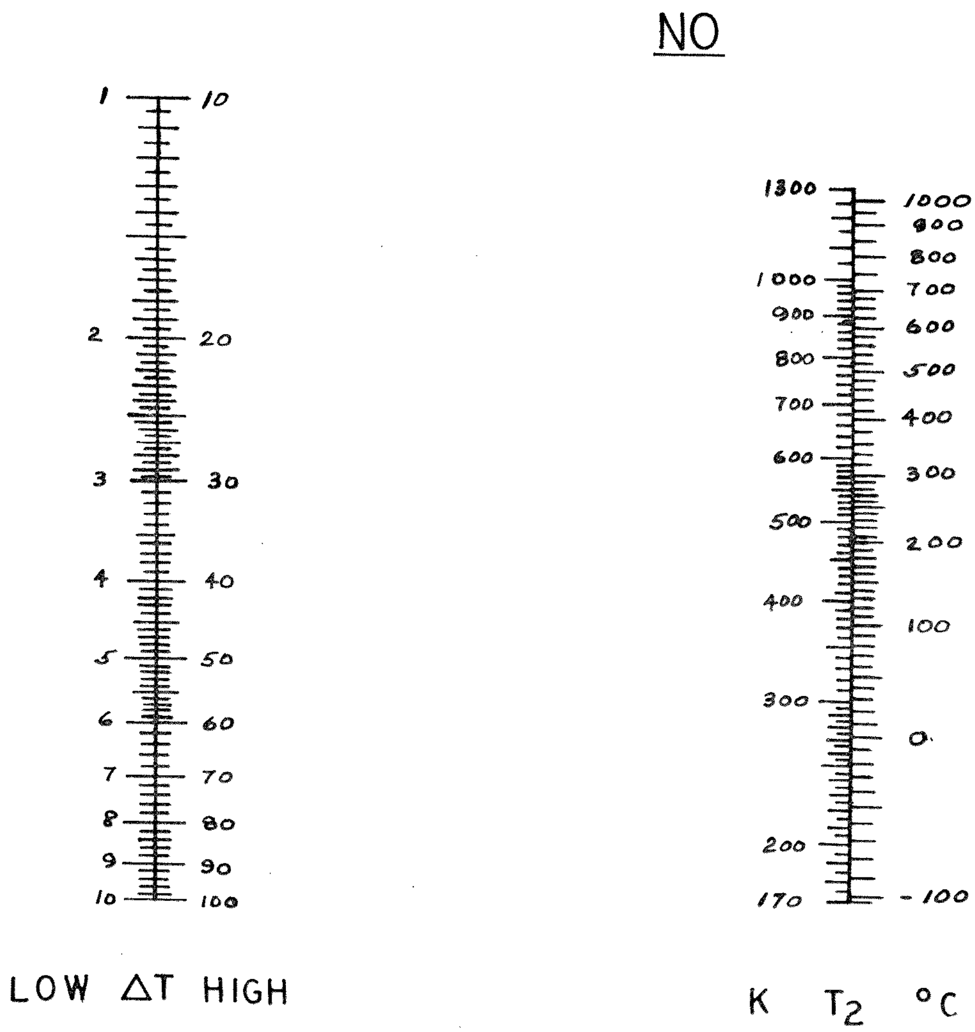
(3) Walter Herbert Burrows, Graphical Techniques for Engineering Computations, Chemical Publishing Co., Inc., New York, 1965.


NO
1
10
2
20
3
30
4
40
5
50
6
60
7
70
8
80
9
90
10
100
LOW ΔT HIGH
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1000
900
800
700
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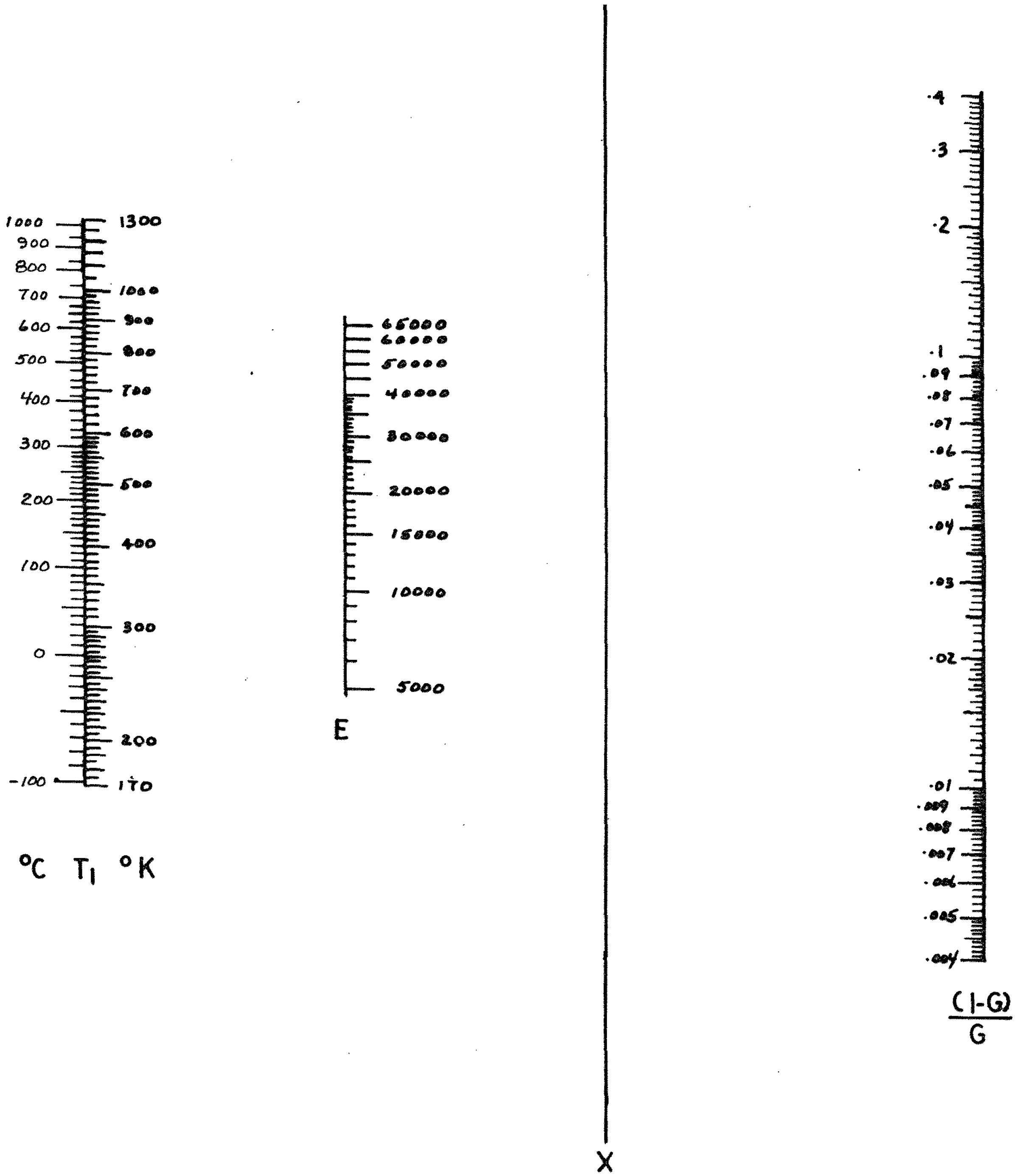
K T2 °C


1000
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30000
20000
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·005
·004
(1-G)/G

The following examples will explain its use.

Example 1

Given: $\Delta t = 50^{o}C$,

$T_1 = 200^{o}C$,

$E = 30,000$ calories per gram mole

Find: k_2/k_1

The nomograph for (1-G)/G is used first. Locate point (1) on the nomograph at $250^{o}C$. Next locate point (2) on the high scale of Δt at Δt equals $50^{o}C$. A straight line is drawn to connect points (1) and (2). The intercept (3) with the (1-G)/G scale is the value for (1-G)/G which is 0.0955.

The nomograph for k_2/k_1 is next used. Locate point (1) on the nomograph at $200^{o}C$. and point (2) at 30,000 calories per gram mole. A straight line is drawn between points (1) and (2) and extended to intersect the pivotal line at point (3). The value of (1-G)/G obtained from the first nomograph is located at point (4). Another straight line is connected between points (3) and (4). The intersection (5) on the k_2/k_1 scale is the value 20.9 which is the solution. This value can be compared with the tabular value of 21.101 and the graphical value of 21.1. The tabular and graphical values are read directly from the graphs and tables in the appendix.

Method	k_2/k_1	% Difference
Table*	21.101	0
Graph	21.1	0
Nomograph	20.9	-1

*The computed value is 21.101

FIGURE 1

NOMOGRAPH FOR (1-G)/G

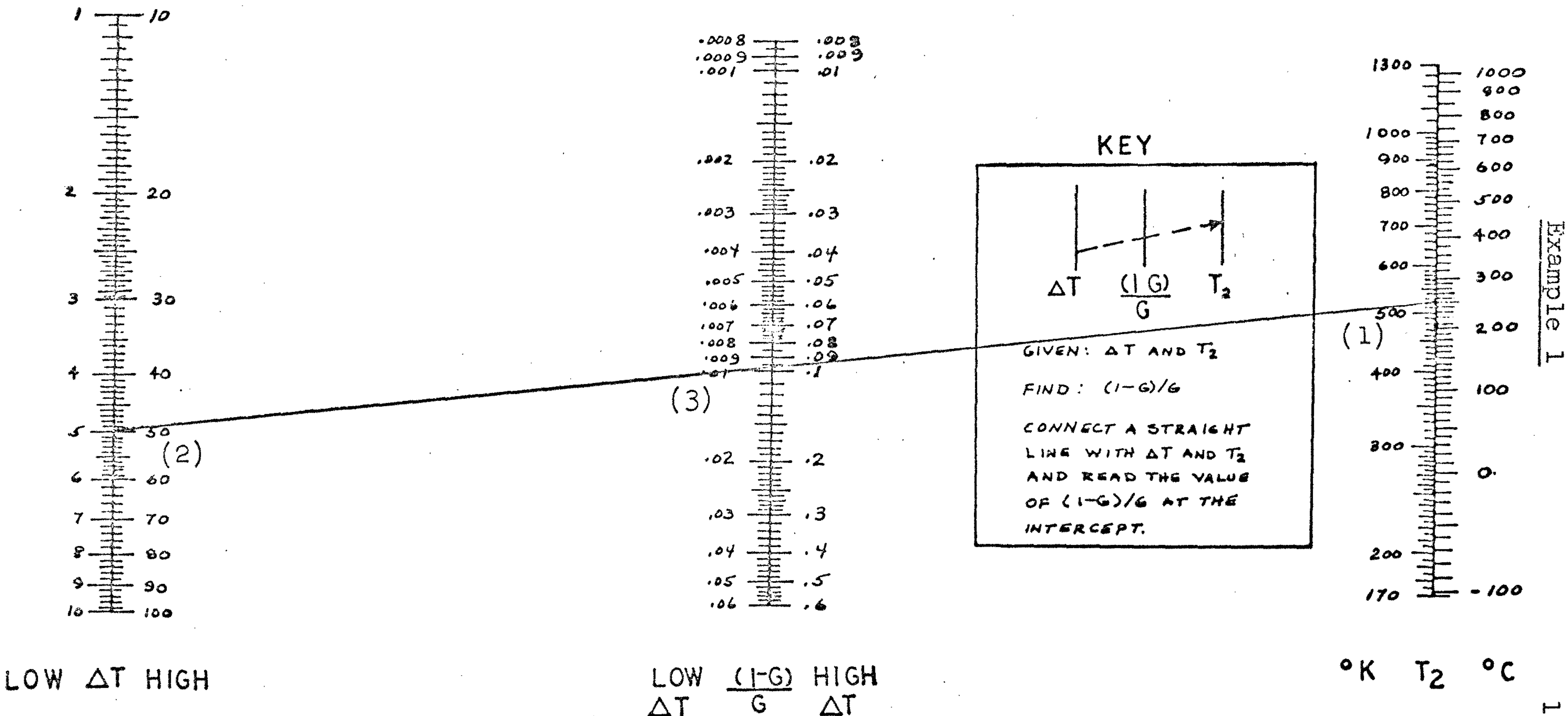
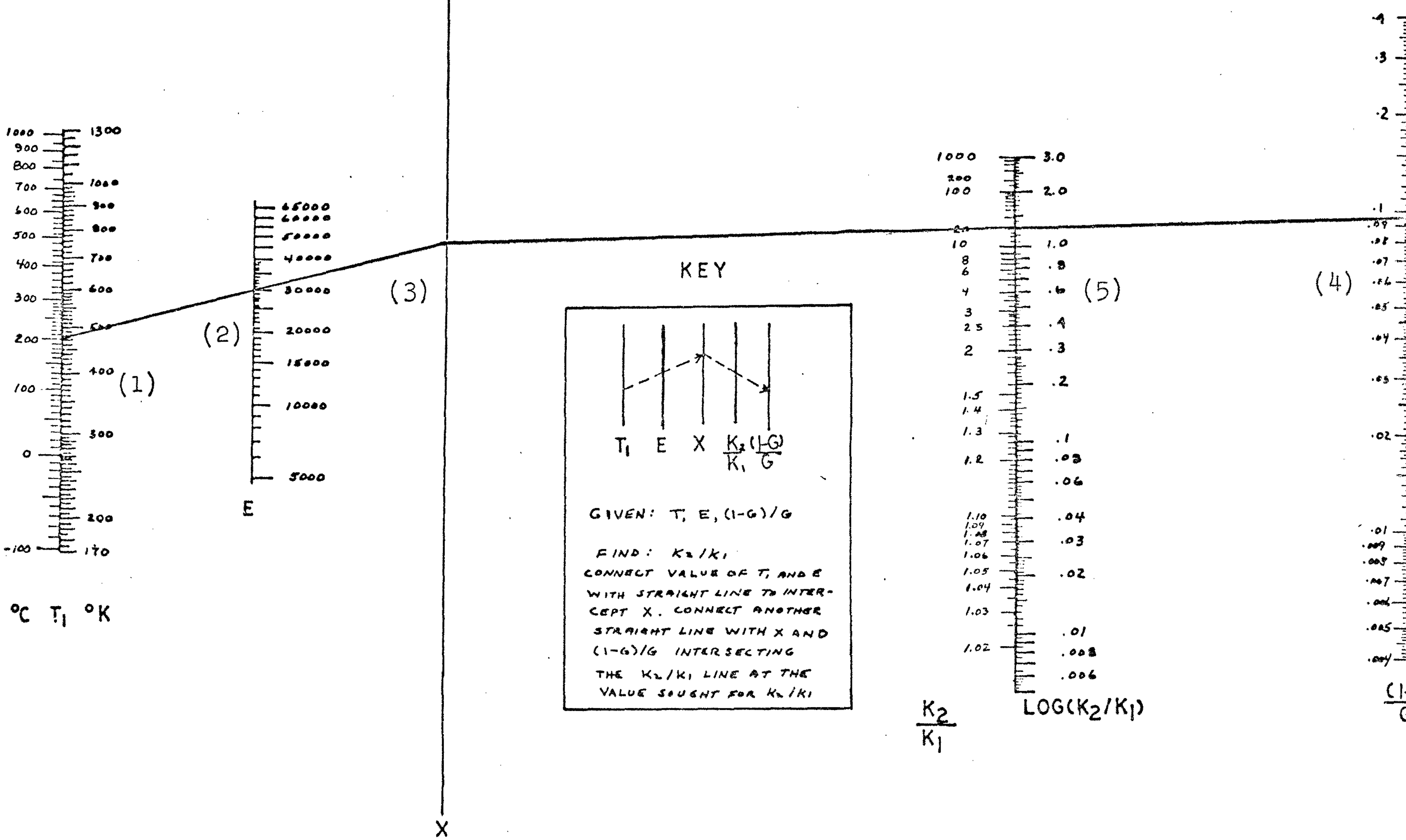


FIGURE 2

NOMOGRAPH FOR K_2/K_1



EXAMPLE 1

Example 2

Given: $k_2/k_1 = 8$,

$\Delta t = 60^{o}C$,

$T_1 = 300^{o}C$.

Find: E

The nomograph for (1-G)/G is used first. Locate point (1) on the nomograph at 360°C. Next locate point (2) on the high scale of Δt at Δt equals 60°C. A straight line is drawn connecting points (1) and (2). The intercept (3) with the (1-G)/G scale is the value for (1-G)/G which is .0975.

The nomograph for k_2/k_1 is next used. Locate point (1) on the nomograph at k_2/k_1 equals 8 and locate point (2) at the value of (1-G)/G obtained from the first nomograph. A straight line connecting points (1) and (2) intersect the pivotal line (X) at point (3). Point (4) is located at 300°C and a straight line is connected between points (3) and (4). The intersection (5) with the E scale is the value of 25250 which is the solution. The nomograph value is compared with the tabular and graphical values below.

Method	E, Calories per Gram Mole	% Difference
Table*	24990	0.
Graph	24900	-0.4
Nomograph	25250	+1

*The correct value is 24990

FIGURE 1

NOMOGRAPH FOR (1-G)/G

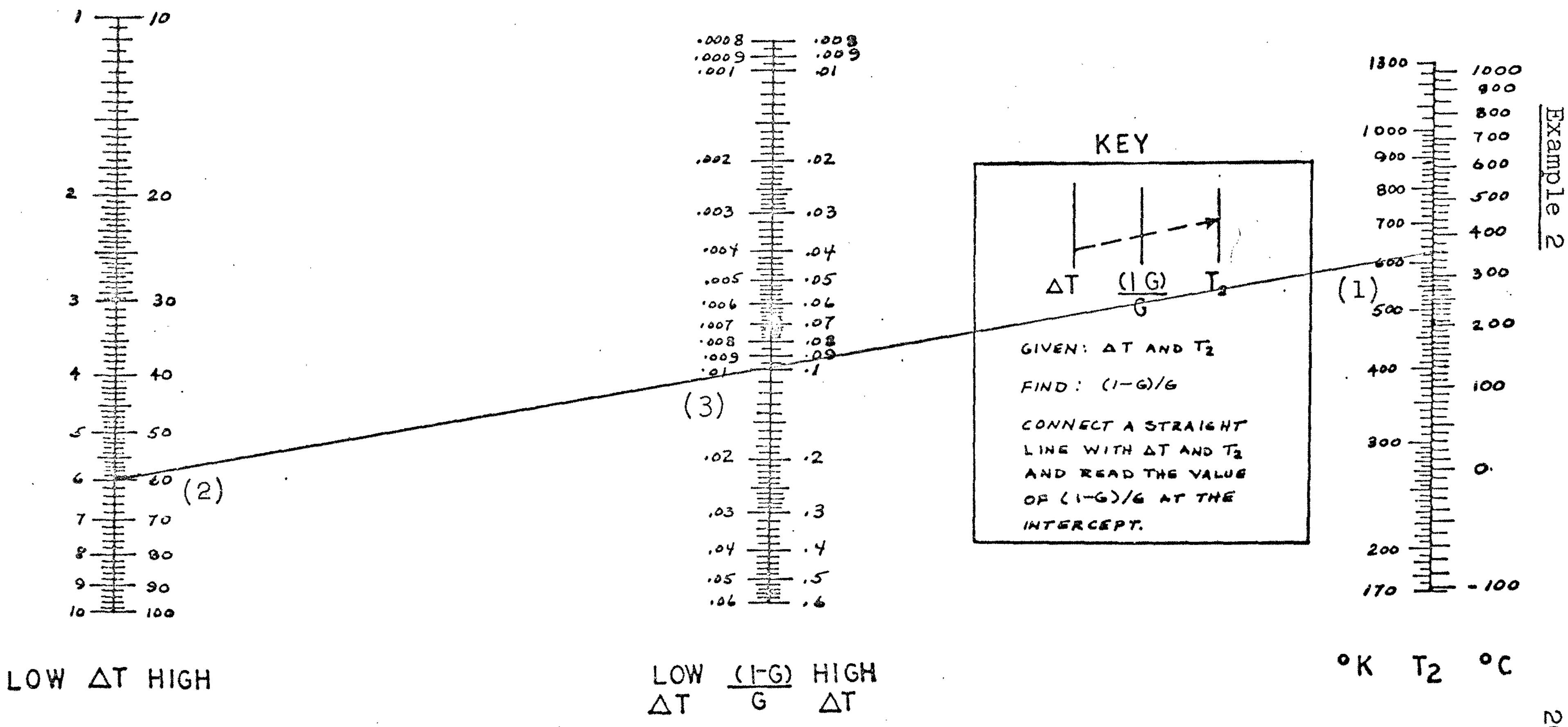
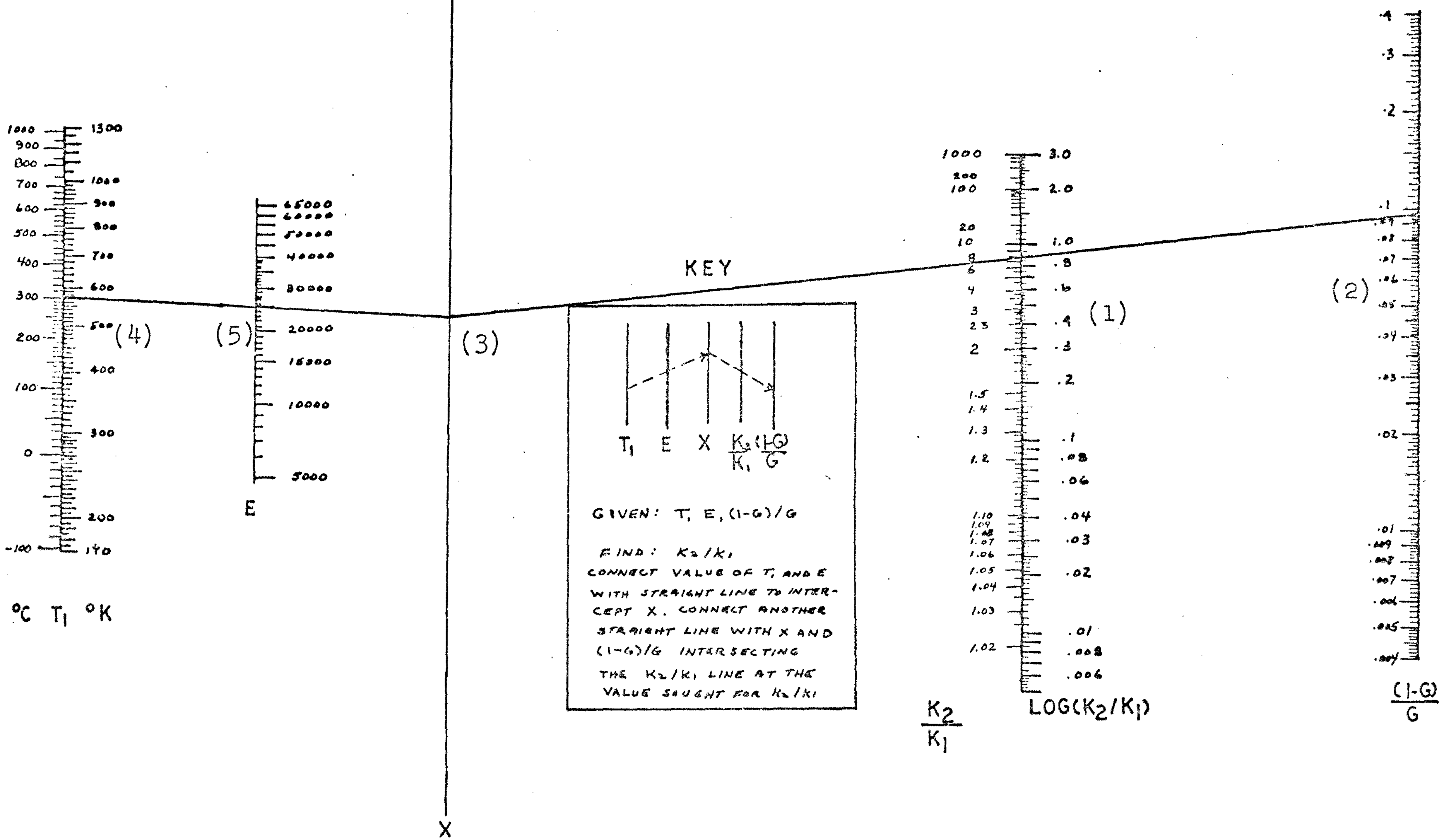


FIGURE 2

NOMOGRAPH FOR K_2/K_1



EXAMPLE 2

Example 3

Given: $E = 40{,}000$ calories per gram mole,

$T_1 = 200°C$

$k_1/k_2 = 5.6$.

Find: Δt.

For this problem the k_2/k_1 nomograph is used first. Locate point (1) at T_1 equal to 200°C and locate point (2) at E equal to 40,000 calories per gram mole. A straight line connecting points (1) and (2) will intersect the pivotal line (X) at point (3). Locate point (4) on the k_2/k_1 scale at 5.6. A straight line connecting points (3) and (4) will intersect the (1-G)/G scale at point (5). The value of (1-G)/G at point (5) is 0.0405. This value of (1-G)/G is then used with the (1-G)/G nomograph to find Δt. Since the nomograph of (1-G)/G is in terms of Δt and T_2 it is necessary to perform a trial and error solution for Δt. The procedure to follow is:

1. Locate point (1) on the (1-G)/G scale with the value found in the k_2/k_1 nomograph.

2. Locate T_1 (200°C) on the T_2 scale at point (2).

3. Connect a straight line between points (1) and (2) locating point (3) on the Δt scale. The value is $19^{o}C$.
4. Add $19^{o}C$ to T_1 and obtain the value of $219^{o}C$. This value is the trial value of T_2.
5. Locate point (4) on the T_2 scale of $219^{o}C$.
6. With a straight line connect points (1) and (4). The intersection on the Δt scale is the new value of Δt which is $19.4^{o}C$.
7. Adding $19.4^{o}C$ to $200^{o}C$ the value of $219.4^{o}C$ for T_2 is obtained.
8. Another trial will essentially give a value of Δt equal to $19.4^{o}C$ which is the answer sought.

The above answers cannot be compared with the table values and graphical values since the answer does not correspond to an exact data point.

FIGURE 2

NOMOGRAPH FOR K_2/K_1

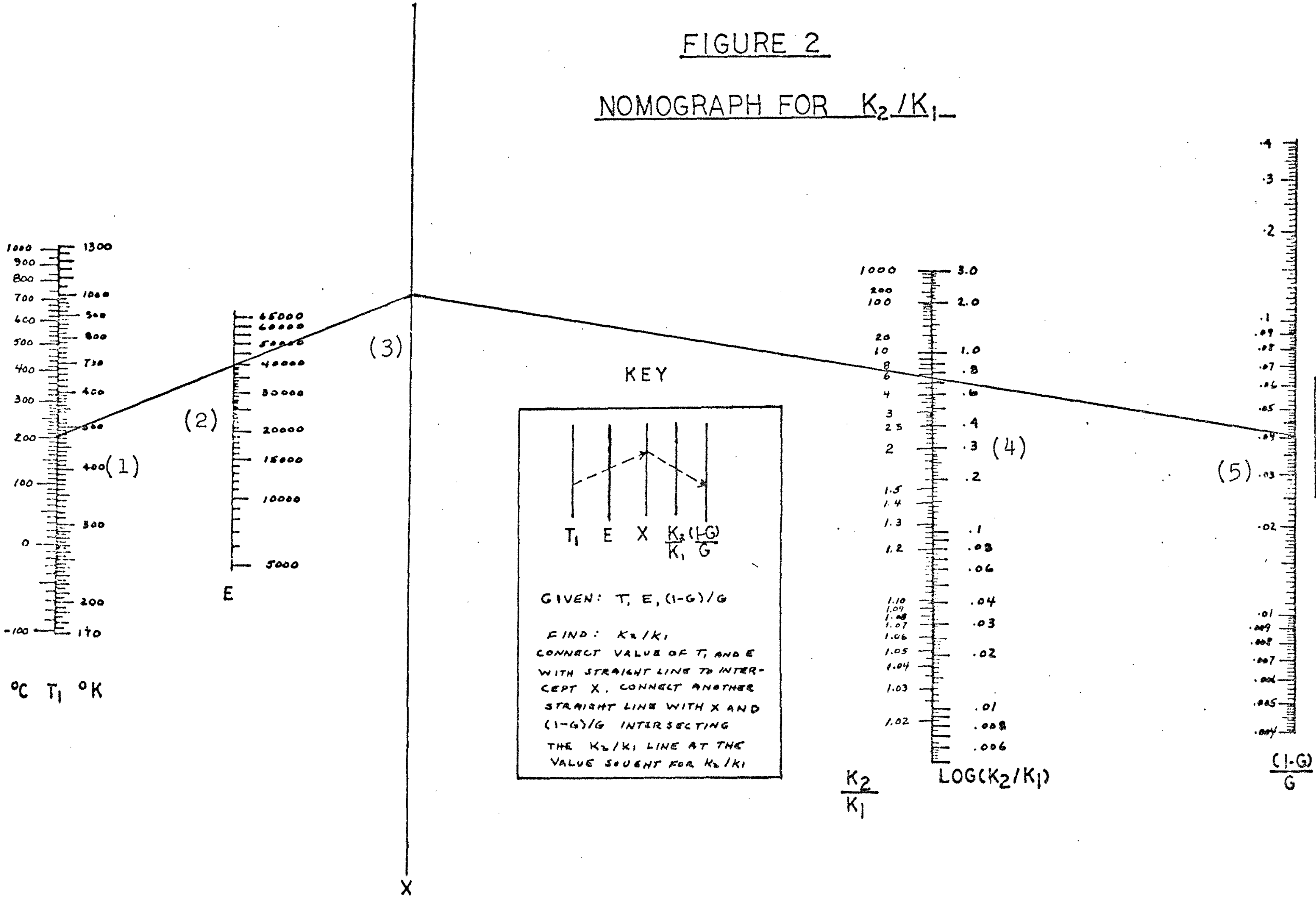
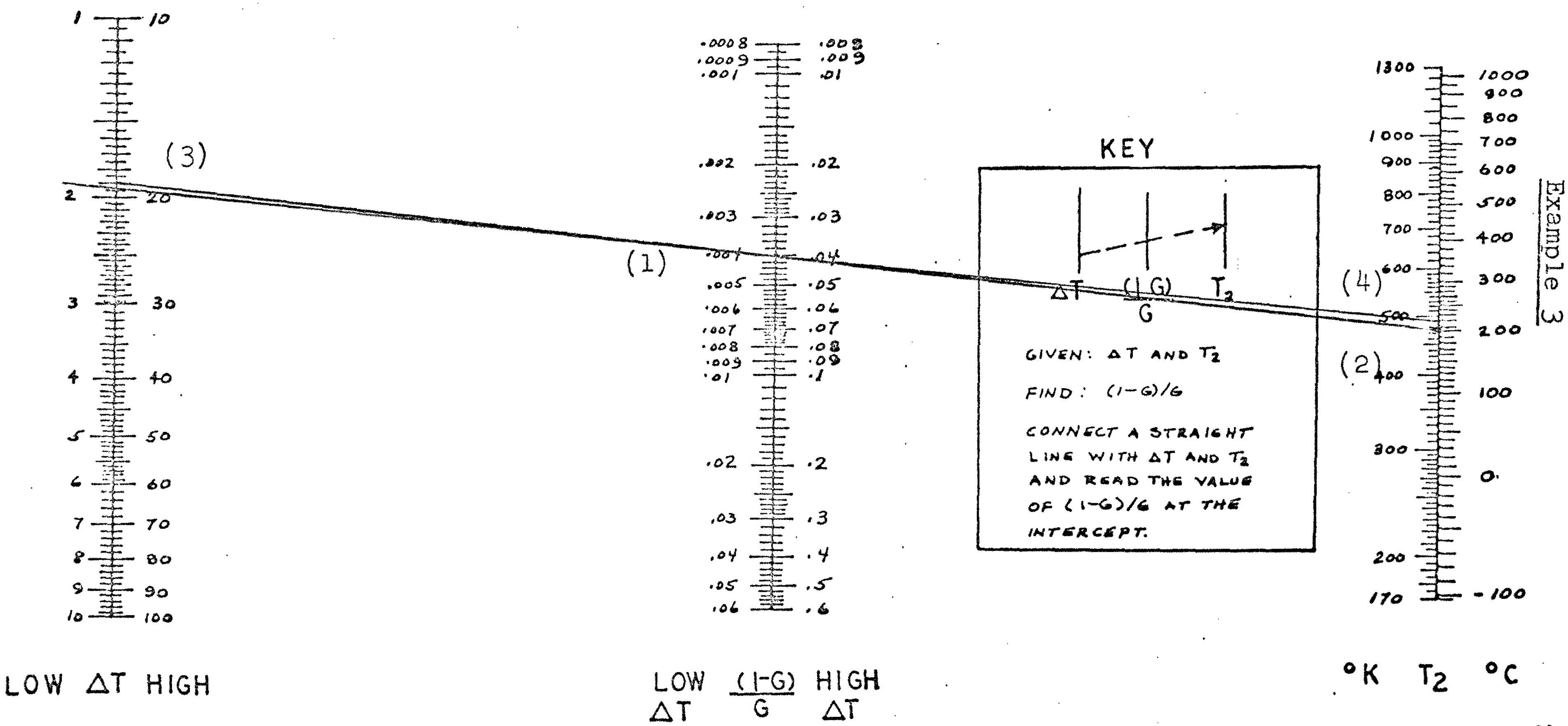


FIGURE 1

NOMOGRAPH FOR (1-G)/G



Example 4

Given: E = 30,000 calories per gram mole,

T_1 = 400°C,

T_2 = 450°C,

k_1 = 3.0.

Find: k_2

The nomograph for (1-G)/G is used first. Locate point (1) on the nomograph at 450°C. Next locate point (2) on the high scale of Δt at Δt equals 50°C. A straight line is drawn connecting points (1) and (2). The intercept (3) with the (1-G)/G scale is the value for (1-G)/G which is .069.

The nomograph for k_2/k_1 is used next. Locate point (1) on the nomograph at T_1 equals 400°C and point (2) at E equals 30,000 calories per gram mole. A straight line connecting points (1) and (2) will intercept the pivotal line (X) at point (3). The value of (1-G)/G is next located at point (4). A straight line connecting points (3) and (4) will intercept the k_2/k_1 scale at point (5) which is 4.69. This value is k_2/k_1. Since k_1 equals 3.0 the value of k_2 is equal to 3.0 times 4.69 or 14.07. The nomograph value is compared with the tabular and graphical values below.

Method	k_2	% Difference
Table*	14.142	0
Graph	14.10	-0.3
Nomograph	14.07	-0.5

*The correct value is 14.142.

FIGURE 1

NOMOGRAPH FOR (1-G)/G

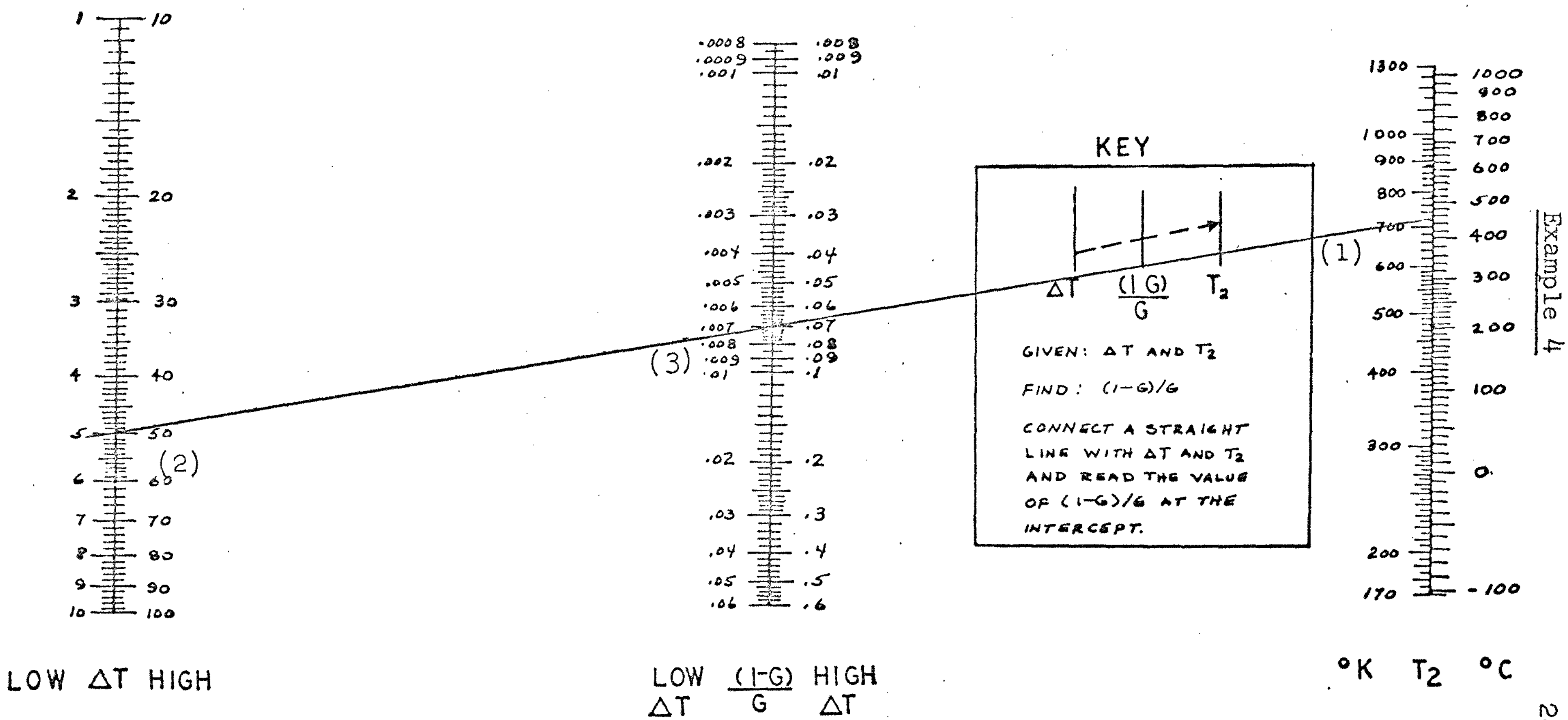
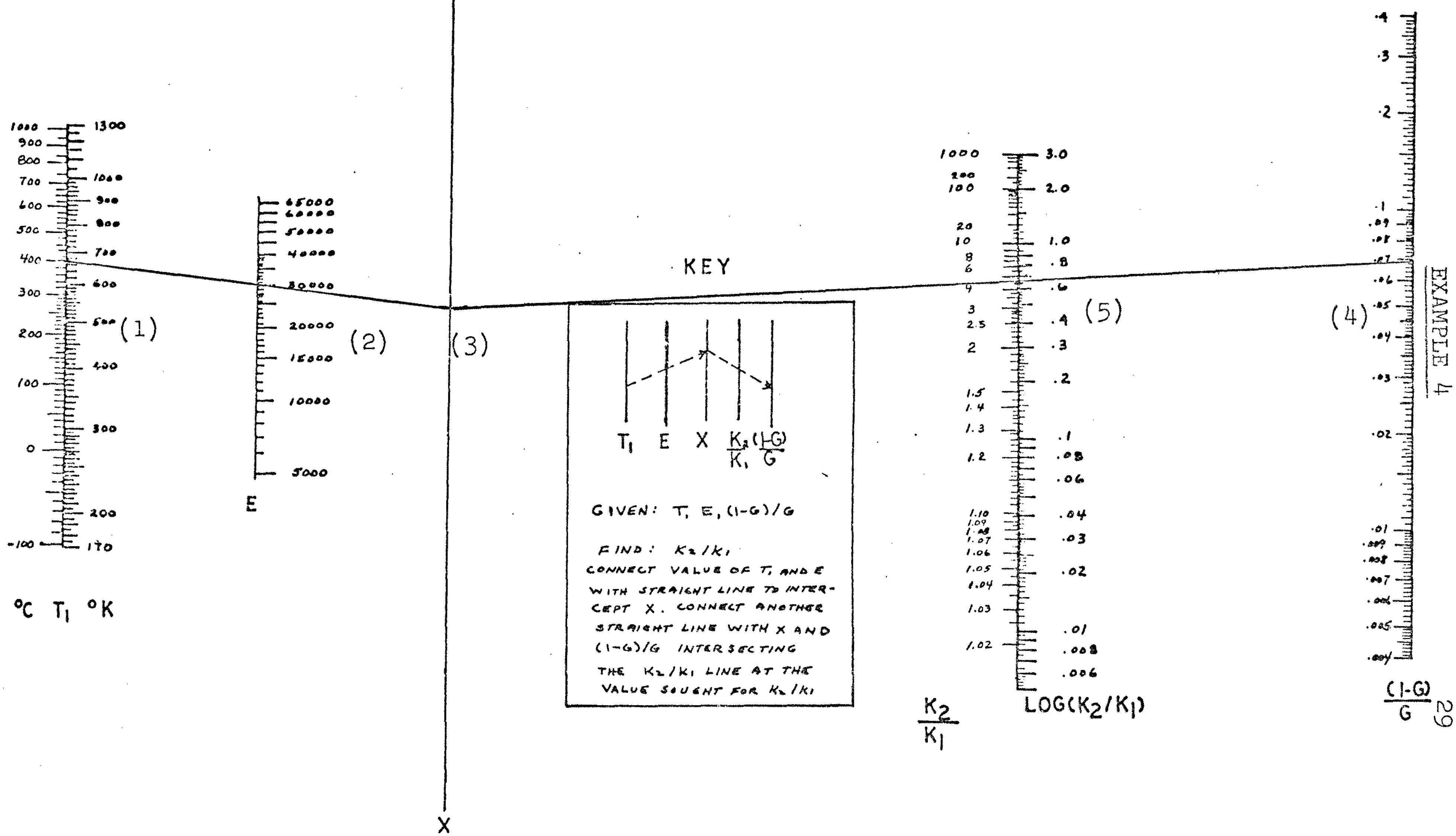


FIGURE 2

NOMOGRAPH FOR K_2/K_1



EXAMPLE 4

CONCLUSIONS

The ideal manner in which to obtain data might be described as the easiest and fastest way consistent with the degree of accuracy sought. To this end, the writer feels that the computational aids presented in this paper fulfill the above description.

The nomograph, graphs, tables and computer programs presented in this paper may be used singly or together to suit the accuracy desired.

Firstly, if the given data corresponds exactly to one of the tables presented it is an easy matter to look up the desired value from the tables in the appendix. If the given data matches the temperatures but not the activation energy the value sought can be easily obtained from the graphs since the activation energies are presented on the abscissa and are continuous from 5,000 to 65,000 calories per gram mole.

Secondly, if the degree of accuracy is not critical the nomograph may be used for all reference temperatures between -100 and 1,000^{o}C, temperature differences between 1 and 100^{o}C and activation energies between 5,000 and 65,000 calories per gram mole. The nomograph is limited to k_2/k_1 values of less than 1,000.

Thirdly, if more accuracy is needed, interpolation with the tables may be done using the nomograph to obtain a multiplication factor in lieu of using logarithms to interpolate.

An example will serve to illustrate the method.

Given: $\Delta t = 50^\circ C$,

$T = 200^\circ C$,

$E = 4{,}000$ calories per gram mole

Find: k_2/k_1

Assuming that the activation energy is located in the table for $200^\circ C$ but that there is no value for Δt equal to $50^\circ C$ obtain k_2/k_1 for the two Δt's bracketing the desired value.

We assume that k_2/k_1 values are available for Δt equal $40^\circ C$ and Δt equal $60^\circ C$. The values of k_2/k_1 then are:

for $T = 200^\circ C$,

$E = 40{,}000$ calories per gram mole,

$\Delta t = 40$,

$k_2/k_1 = 27.551$.

and for $T = 200^{\circ}C$,

$E = 40{,}000$ calories per gram mole,

$\Delta t = 60^{\circ}C$,

$k_2/k_1 = 119.997$

It is obvious that for this problem direct interpolation would result in a value of k_2/k_1, at $\Delta t = 50^{\circ}C$, of 73.774. This result is wrong, the correct value being 58.312.

However, we may use the nomograph to obtain a multiplication factor M such that:

$$\left(\frac{k_2}{k_1}\right)_{t=50^{\circ}C} = \left(\frac{k_2}{k_1}\right)_{t=40^{\circ}C} + M\left[\left(\frac{k_2}{k_1}\right)_{t=60^{\circ}C} - \left(\frac{k_2}{k_1}\right)_{t=40^{\circ}C}\right] \quad (3\text{-}1)$$

This would be accomplished by using the nomograph to obtain the k_2/k_1 values for the above conditions. The values obtained would be:

$$(k_2/k_1) \quad t = 40 = 28$$

$$(k_2/k_1) \quad t = 60 = 120.$$

Also a value would be determined with the nomograph for the value of (k_2/k_1) at $\Delta t = 50^{\circ}C$ which would be 58. The value of M would then be:

$$58 = 28 + M\ (120-28)$$

$$M = \frac{30}{92} = 0.326$$

Using the above factor with the table values we obtain:

$$(k_2/k_1)_{\Delta t=50^\circ C} = 27.551 + .326(119.997 - 27.551)$$

$$(k_2/k_1)_{\Delta t=50^\circ C} = 27.551 + .326(92.446)$$

$$(k_2/k_1)_{\Delta t=50^\circ C} = 27.551 + 30.131$$

$$(k_2/k_1)_{\Delta t=50^\circ C} = 57.682$$

which compares favorably with the computer value of 58.312 the error being slightly more than one per cent.

RECOMMENDATIONS

Since computational aids for the calculation of the Arrhenius equation have not been presented before it is hoped that refinements to the material presented in this paper will be made in the future.

The nomograph k_2/k_1 as presented in this paper encompasses a relatively large range of temperatures and activation energies. Future studies could be made in constructing nomographs with narrower ranges of temperature, activation energies or k_2/k_1 values. The resultant nomographs would be relatively larger and finer graduations could be obtained.

An alternate approach to additional work would be to utilize the computer to construct tables of k_2/k_1 as a function of activation energies and temperatures and provide interpolation factors to be used for intermediate data points.

Lastly, graphs of k_2/k_1 could also be constructed with a correlation between graphs to facilitate interpolation.

APPENDIX

Program 1

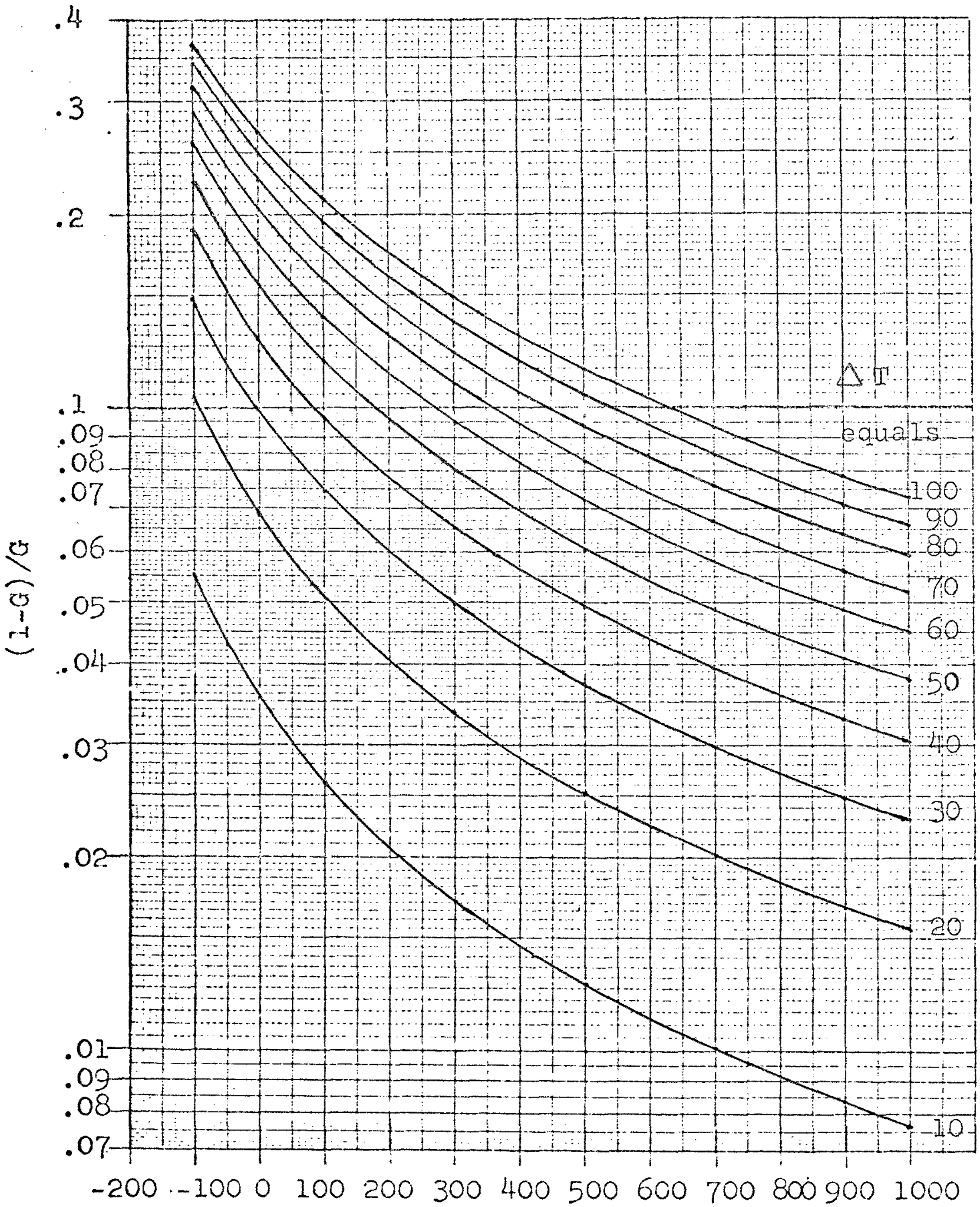
Program for the Calculation of the Value (1-G)/G

```
C THIS PROGRAM CALCULATES THE VALUE OF (1-G)/G FOR
C A REFERENCE TEMPERATURE OF -100 TO 1000 DEG C
C IN INCREMENTS OF 50 DEG C. AT A DELTA TEMPERATURE
C 1-10 FOR REF TEMP OF -100 TO 300 DEG C. AND
C 10-100 FOR REF TEMP OF -100 TO 1000 DEG C.
      DIMENSION IP(100),G(100)
C SUPPLY DATA FOR EACH TABLE
C L=SUBTRACT. CONST. FOR TEMP BELOW 0 DEG C.
C KI,KM,KT=DO LOOP INDEX FOR REF TEMP
C JI,JM,JT=DO LOOP INDEX FOR DELTA TEMP
C N=TABLE NUMBER
   30 READ (2,100) L,KI,KM,KT,JI,JM,JT,N
C EXIT TEST, LAST DATA CARD ALL ZERO'S
      IF (KI) 40,50,40
C PRINT TABLE NO.
   40 WRITE (5,200) N
C OBTAIN DELTA TEMP
      DO 15 J= JI,JM,JT
      IP(J) = J
   15 CONTINUE
C PRINT DELTA TEMP HEADING
      WRITE (5,300)
      WRITE (5,400) (IP(J),J = JI,JM,JT)
C CALCULATE TEMP 2
      DO 10 K=KI,KM,KT
      M = L + K
      T1A = M + 273.16
C CALCULATE (1-G)/G = DELTA T/T2
      DO 20 J = JI,JM,JT
      O = M + J
      T2A = O + 273.16
      G(J) = (T1A - T2A)/T2A
   20 CONTINUE
C PRINT REF TEMP AND (1-G)/G FOR DELTA TEMPERATURES
      WRITE (5,500) M,(G(J),J = JI,JM,JT)
   10 CONTINUE
C GO TO NEXT DATA CARD FOR NEW TABLE
      GO TO 30
  100 FORMAT (8I4)
  200 FORMAT (1H1///////////////48X,'TABLE NO. ',I2,' VAL
     1UES OF (1-G)/G'/////)
  300 FORMAT (1H+,45X,'VALUES OF (1-G)/G FOR DELTA TEMPER
```

```
   1ATURE IN DEG C EQUAL TO'//)
400 FORMAT (1H+,14X,'REFERENCE TEMP.       ',10(2X,I3,3X)/
   1//)
500 FORMAT (1H+,20X,I4,10X,10(1X,F7.4)/)
 50 CALL EXIT
    END
```

Figure 3

(1-G)/G for Values of Delta T of 10-100°C



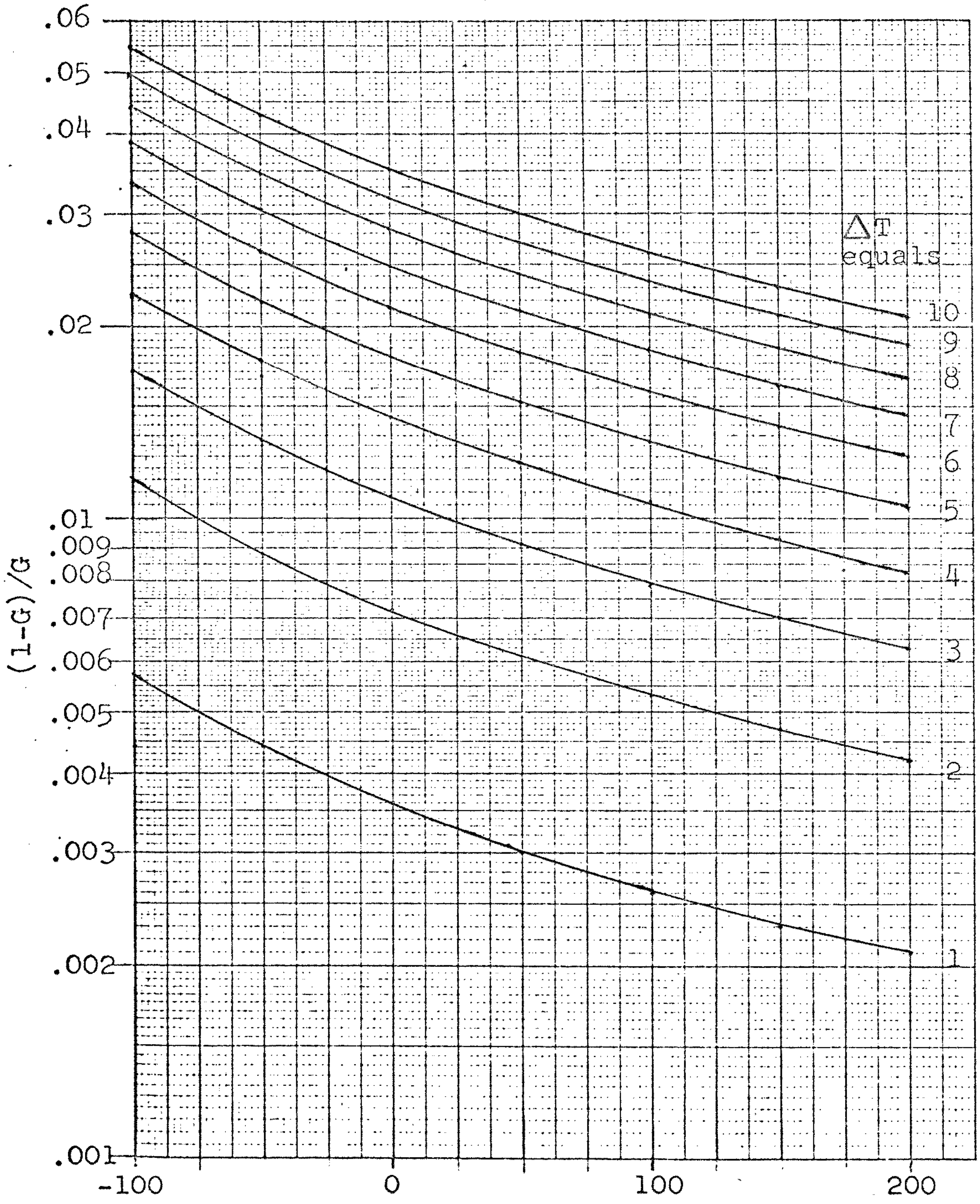
T_1, Temperature in Degrees C

TABLE NO. 24 VALUES OF (1-G)/G

REFERENCE TEMP.	VALUES OF (1-G)/G FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	10	20	30	40	50	60	70	80	90	100
-100	-0.0545	-0.1035	-0.1476	-0.1876	-0.2240	-0.2573	-0.2878	-0.3160	-0.3419	-0.3660
-50	-0.0428	-0.0822	-0.1185	-0.1519	-0.1830	-0.2118	-0.2387	-0.2638	-0.2873	-0.3094
0	-0.0353	-0.0682	-0.0989	-0.1277	-0.1547	-0.1800	-0.2039	-0.2265	-0.2478	-0.2679
50	-0.0300	-0.0582	-0.0849	-0.1101	-0.1339	-0.1565	-0.1780	-0.1984	-0.2178	-0.2363
100	-0.0260	-0.0508	-0.0744	-0.0968	-0.1181	-0.1385	-0.1579	-0.1765	-0.1943	-0.2113
150	-0.0230	-0.0451	-0.0662	-0.0863	-0.1056	-0.1241	-0.1419	-0.1589	-0.1753	-0.1911
200	-0.0206	-0.0405	-0.0596	-0.0779	-0.0955	-0.1125	-0.1288	-0.1446	-0.1598	-0.1744
250	-0.0187	-0.0368	-0.0542	-0.0710	-0.0872	-0.1028	-0.1180	-0.1326	-0.1467	-0.1604
300	-0.0171	-0.0337	-0.0497	-0.0652	-0.0802	-0.0947	-0.1088	-0.1224	-0.1357	-0.1485
350	-0.0157	-0.0310	-0.0459	-0.0603	-0.0742	-0.0878	-0.1009	-0.1137	-0.1261	-0.1382
400	-0.0146	-0.0288	-0.0426	-0.0560	-0.0691	-0.0818	-0.0941	-0.1062	-0.1179	-0.1293
450	-0.0136	-0.0269	-0.0398	-0.0524	-0.0646	-0.0766	-0.0882	-0.0996	-0.1106	-0.1214
500	-0.0127	-0.0252	-0.0373	-0.0491	-0.0607	-0.0720	-0.0830	-0.0937	-0.1042	-0.1145
550	-0.0120	-0.0237	-0.0351	-0.0463	-0.0572	-0.0679	-0.0783	-0.0885	-0.0985	-0.1083
600	-0.0113	-0.0223	-0.0332	-0.0438	-0.0541	-0.0642	-0.0742	-0.0839	-0.0934	-0.1027
650	-0.0107	-0.0212	-0.0314	-0.0415	-0.0513	-0.0610	-0.0704	-0.0797	-0.0888	-0.0977
700	-0.0101	-0.0201	-0.0299	-0.0394	-0.0488	-0.0580	-0.0671	-0.0759	-0.0846	-0.0931
750	-0.0096	-0.0191	-0.0284	-0.0376	-0.0465	-0.0553	-0.0640	-0.0725	-0.0808	-0.0890
800	-0.0092	-0.0182	-0.0271	-0.0359	-0.0445	-0.0529	-0.0612	-0.0693	-0.0773	-0.0852
850	-0.0088	-0.0174	-0.0260	-0.0343	-0.0426	-0.0507	-0.0586	-0.0664	-0.0741	-0.0817
900	-0.0084	-0.0167	-0.0249	-0.0329	-0.0408	-0.0486	-0.0563	-0.0638	-0.0712	-0.0785
950	-0.0081	-0.0160	-0.0239	-0.0316	-0.0392	-0.0467	-0.0541	-0.0613	-0.0685	-0.0755
1000	-0.0077	-0.0154	-0.0230	-0.0304	-0.0377	-0.0450	-0.0521	-0.0591	-0.0660	-0.0728

Figure 4

(1-G)/G for Values of Delta T of 1-10°C



T_1, Temperature in Degrees C

TABLE NO. 25 VALUES OF (1-G)/G

REFERENCE TEMP.	VALUES OF (1-G)/G FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	1	2	3	4	5	6	7	8	9	10
-100	-0.0057	-0.0114	-0.0170	-0.0225	-0.0280	-0.0334	-0.0388	-0.0441	-0.0494	-0.0545
-50	-0.0044	-0.0088	-0.0132	-0.0176	-0.0219	-0.0261	-0.0304	-0.0346	-0.0387	-0.0428
0	-0.0036	-0.0072	-0.0108	-0.0144	-0.0179	-0.0214	-0.0249	-0.0284	-0.0318	-0.0353
50	-0.0030	-0.0061	-0.0091	-0.0122	-0.0152	-0.0182	-0.0212	-0.0241	-0.0270	-0.0300
100	-0.0026	-0.0053	-0.0079	-0.0106	-0.0132	-0.0158	-0.0184	-0.0209	-0.0235	-0.0260
150	-0.0023	-0.0047	-0.0070	-0.0093	-0.0116	-0.0139	-0.0162	-0.0185	-0.0208	-0.0230
200	-0.0021	-0.0042	-0.0063	-0.0083	-0.0104	-0.0125	-0.0145	-0.0166	-0.0186	-0.0206

Figure 5

k_2/k_1

Reference Temperature T1 = -100°C

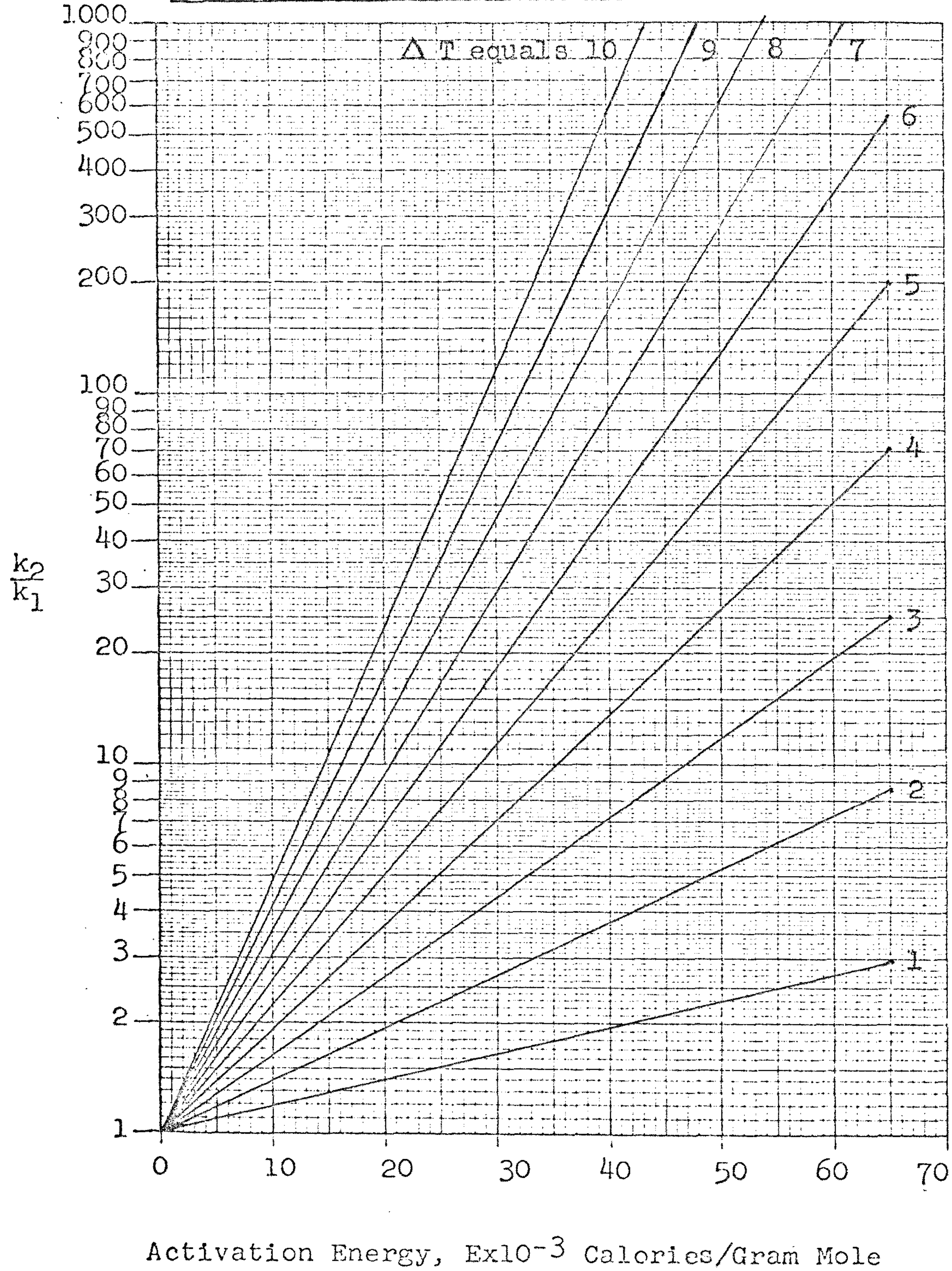
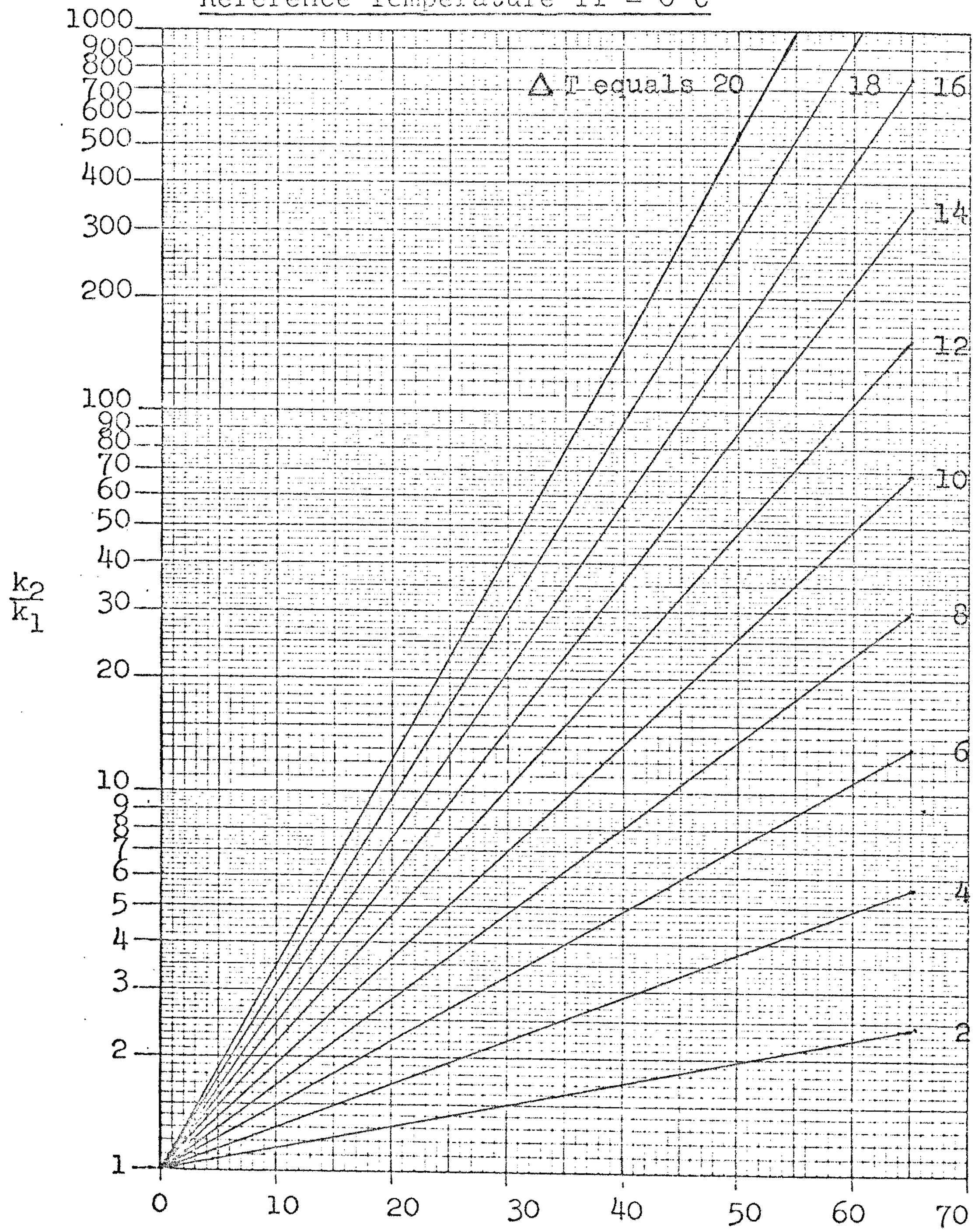


Figure 6

k_2/k_1

Reference Temperature T1 = 0°C

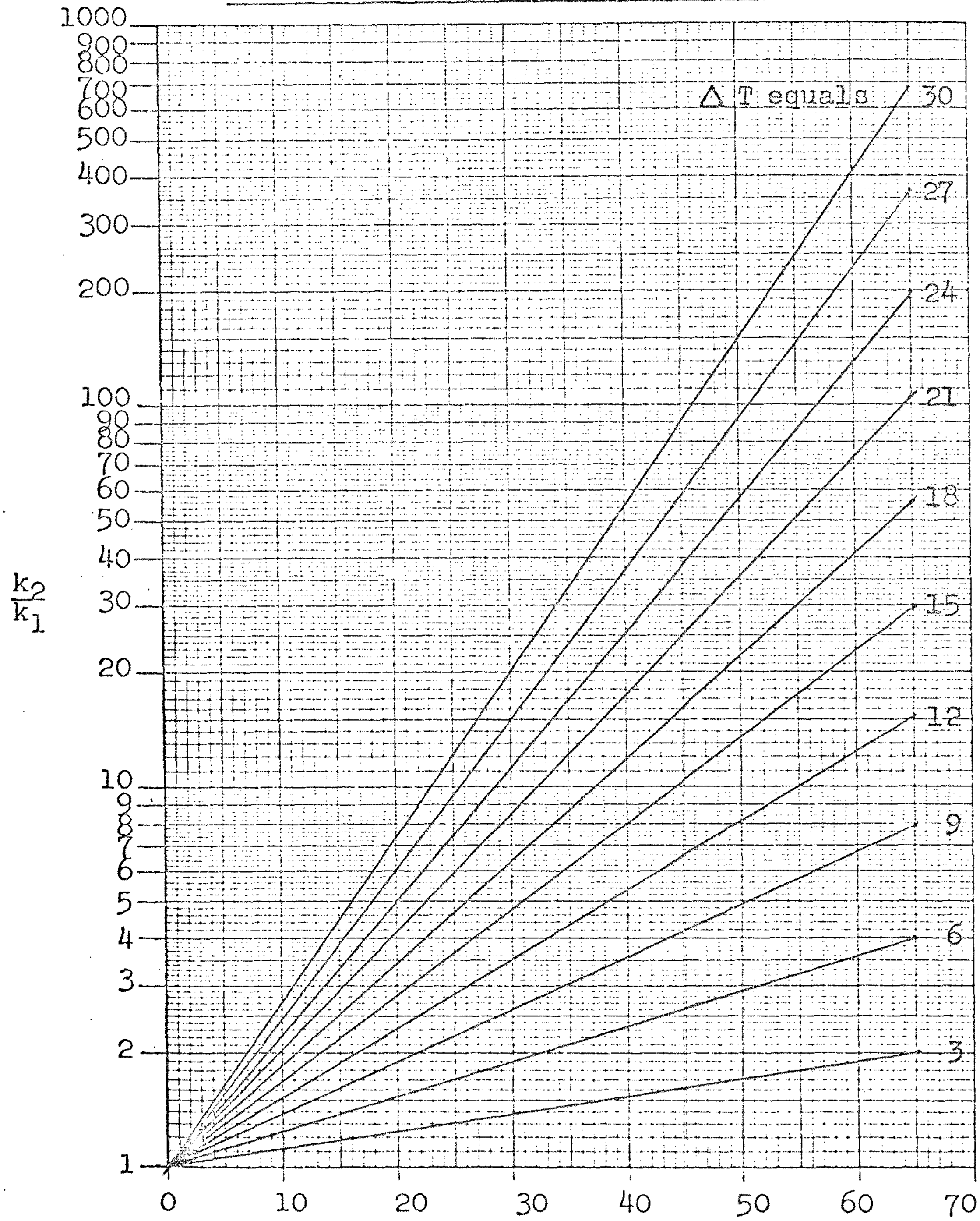


Activation Energy, Ex10^{-3} Calories/Gram Mole

Figure 7

k_2/k_1

Reference Temperature T1 = 100°C



Activation Energy, Ex10^{-3} Calories/Gram Mole

Figure 8

k_2/k_1

Reference Temperature T1 = 200°C

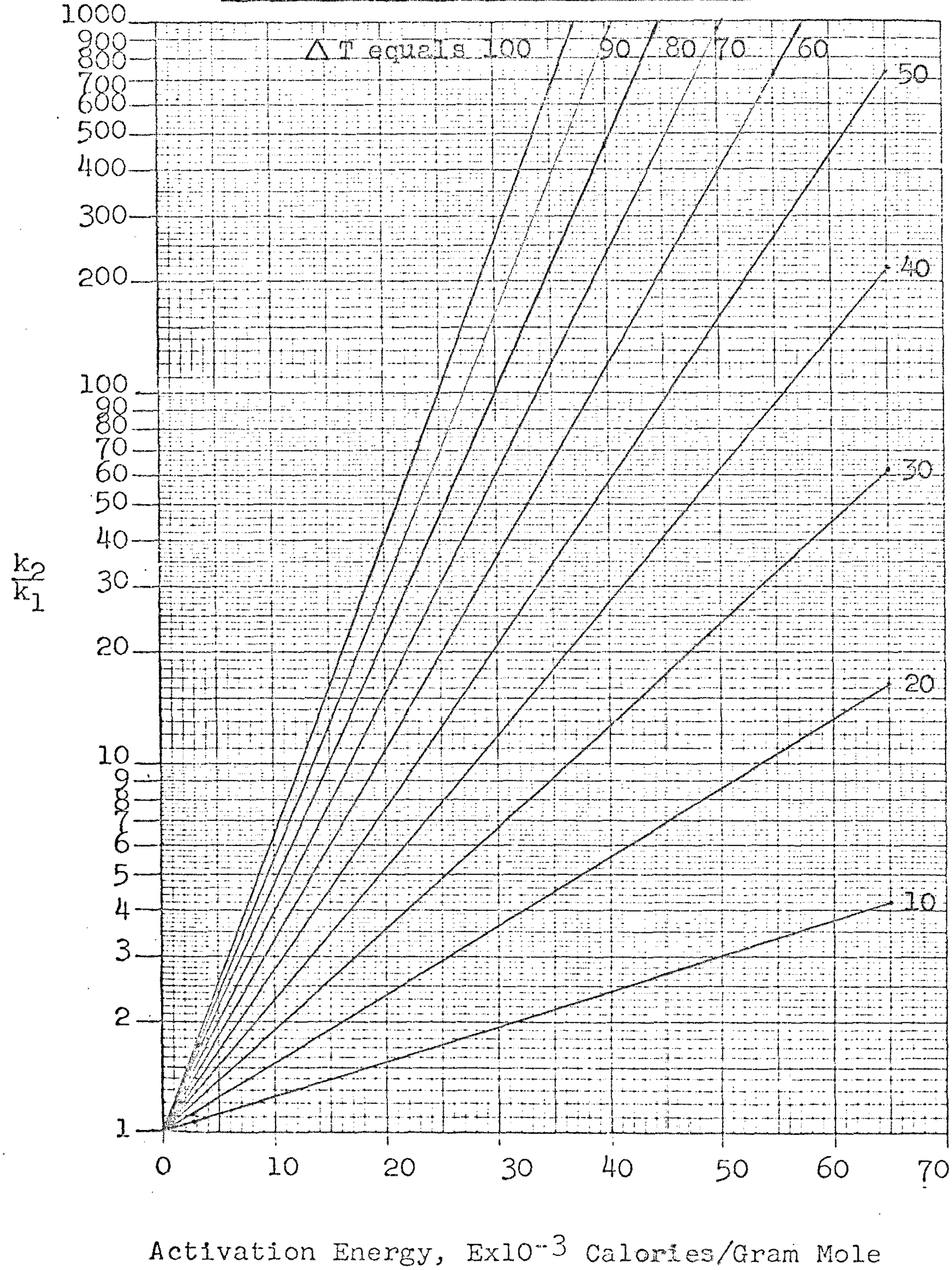
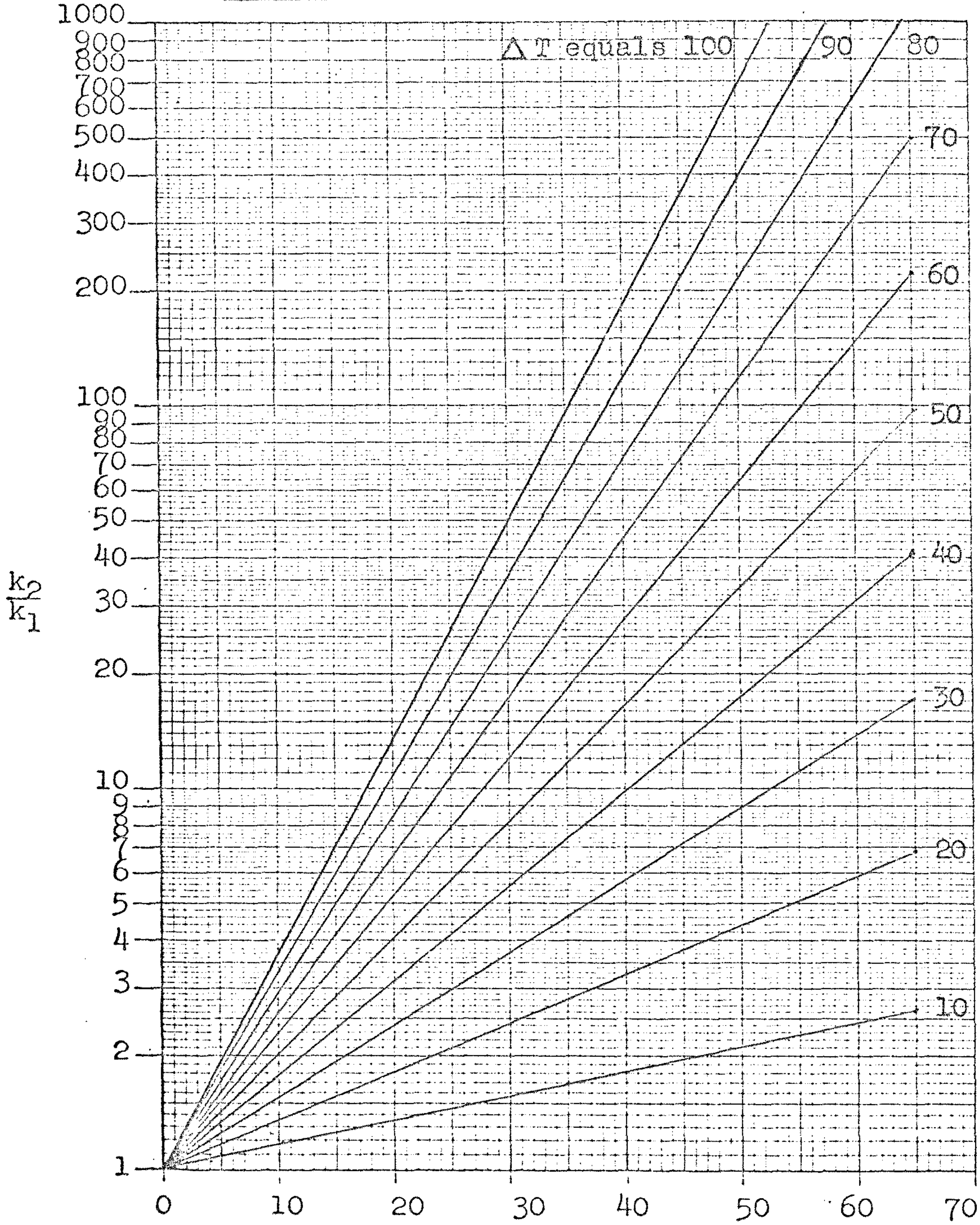


Figure 9

k_2/k_1

Reference Temperature T1 = 300°C

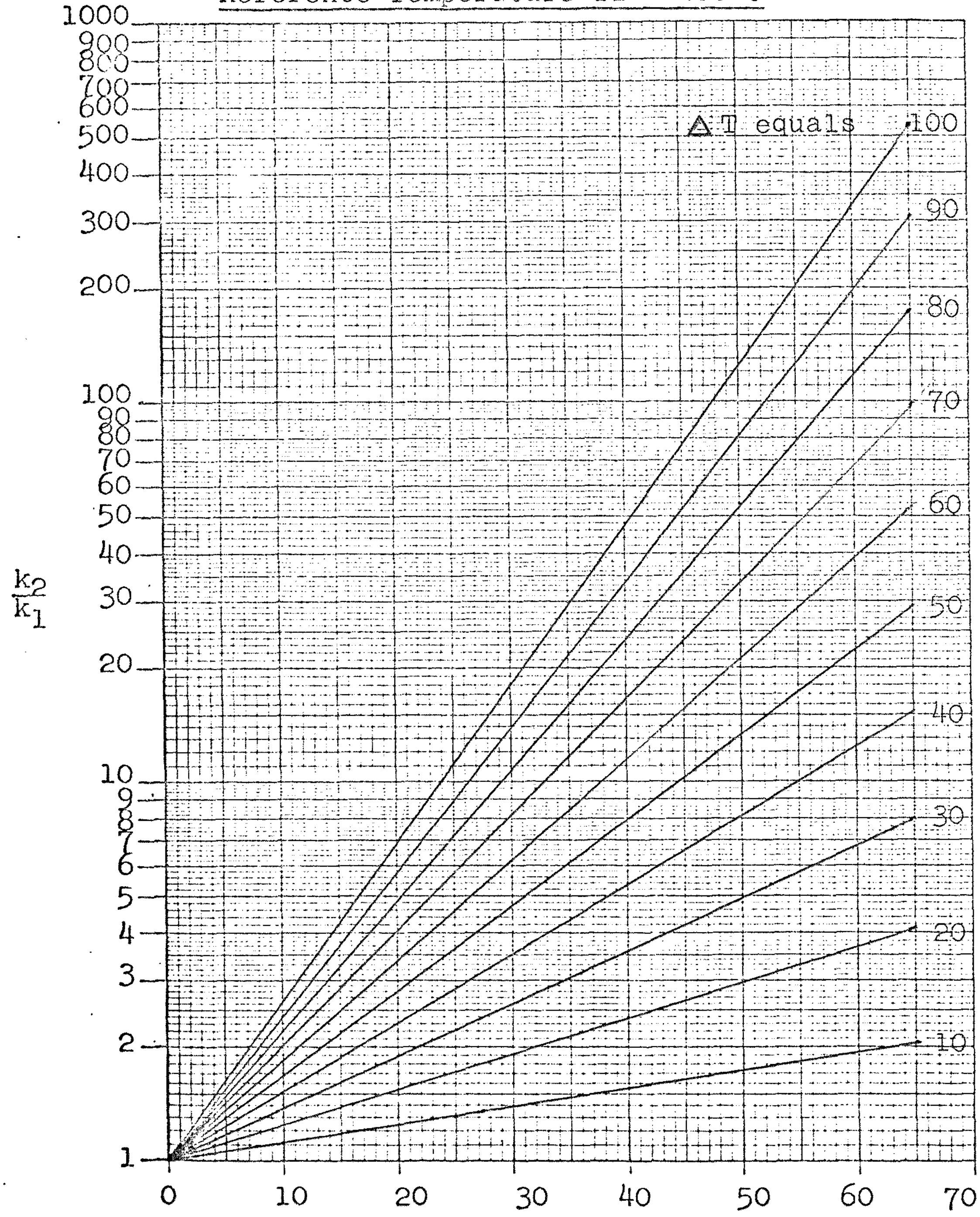


Activation Energy, Ex10^{-3} Calories/Gram Mole

Figure 10

k_2/k_1

Reference Temperature T1 = 400°C

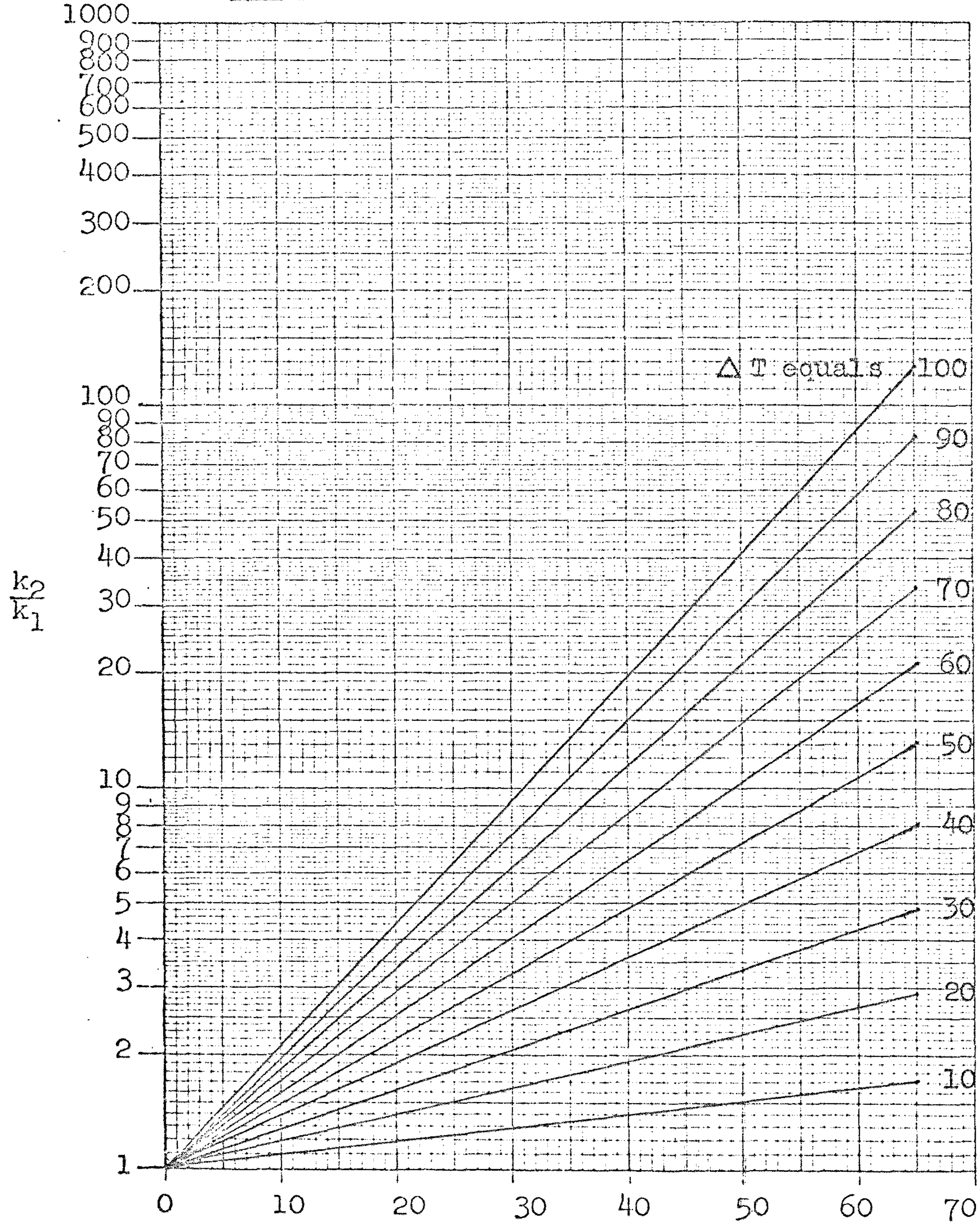


Activation Energy, Ex10^{-3} Calories/Gram Mole

Figure 11

k_2/k_1

Reference Temperature T1 = 500°C

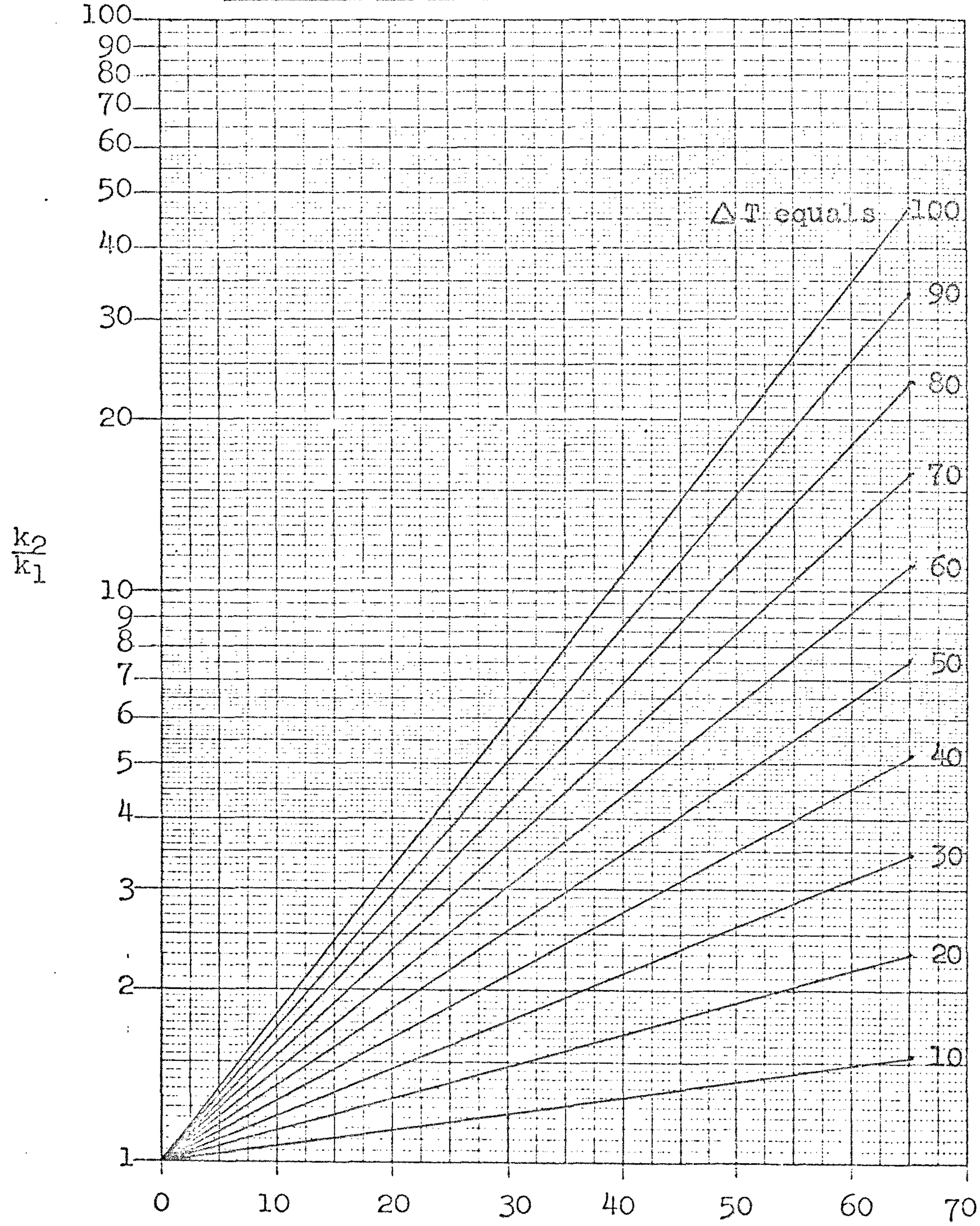


Activation Energy, Ex10^{-3} Calories/Gram Mole

Figure 12

k_2/k_1

Reference Temperature T1 = 600°C



Activation Energy, Ex10^{-3} Calories/Gram Mole

Figure 13

k_2/k_1

Reference Temperature T1 = 700°C

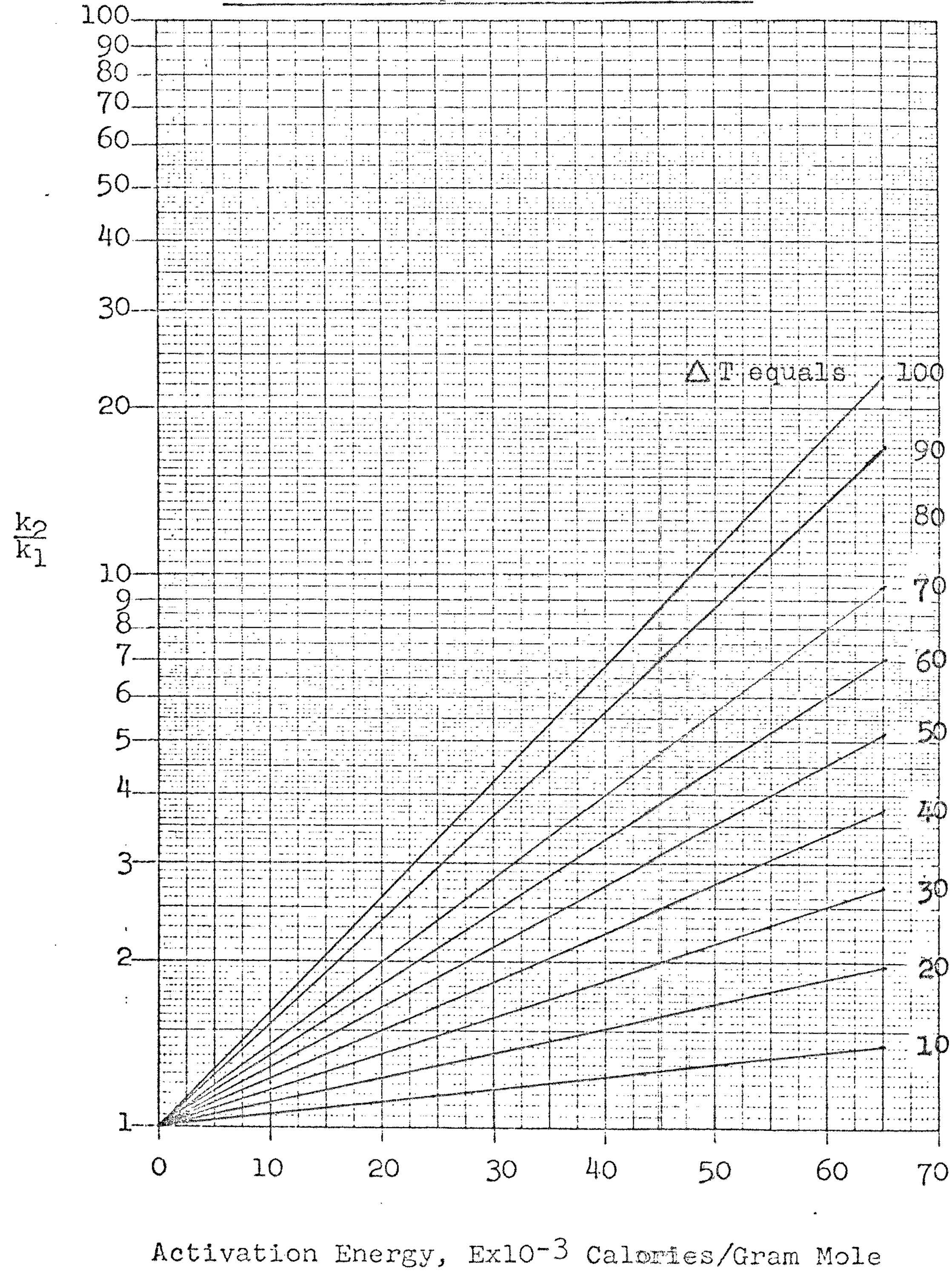


Figure 14

k_2/k_1

Reference Temperature T1 = 800°C

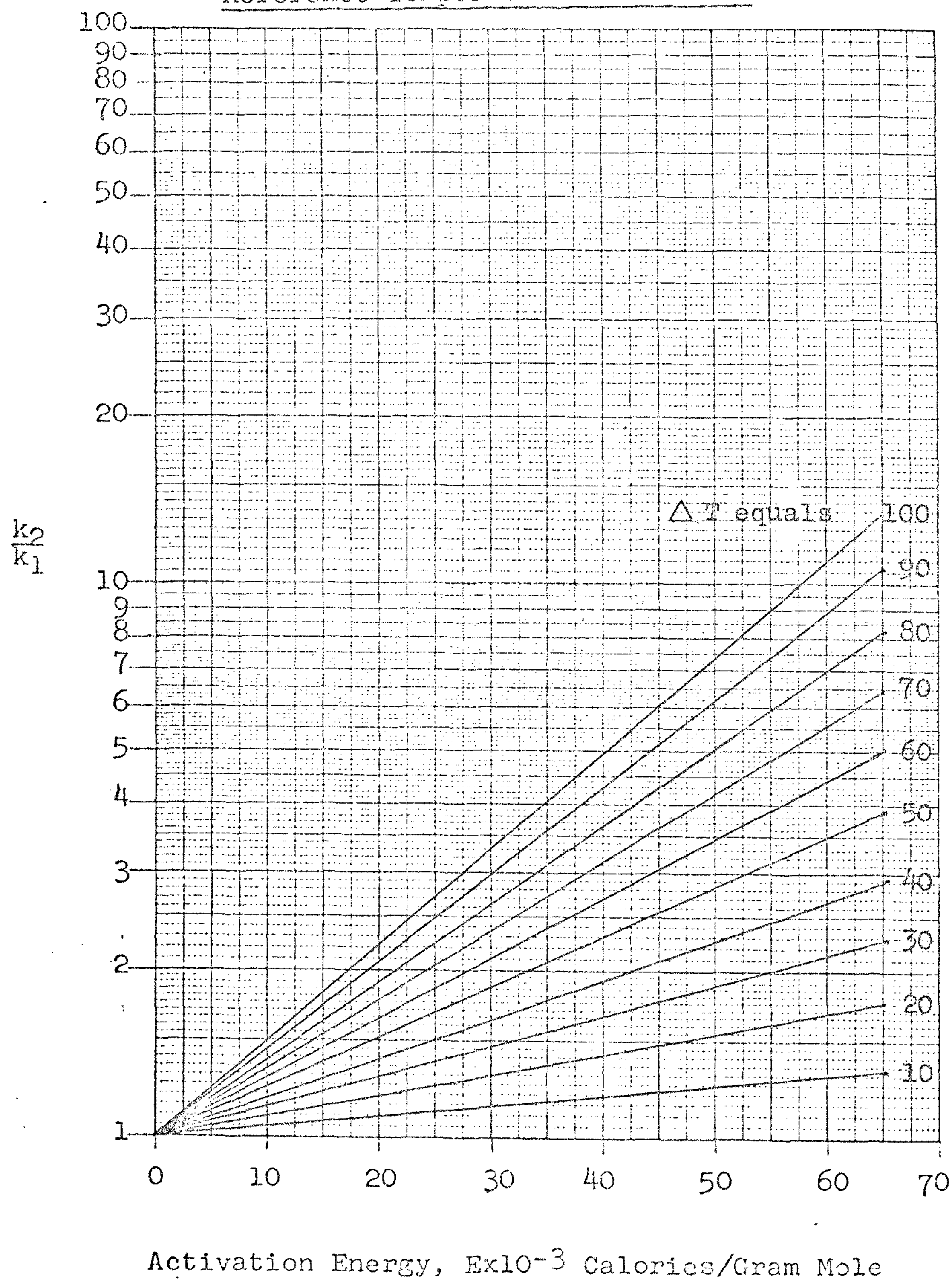


Figure 15

k_2/k_1

Reference Temperature T1 = 900°C

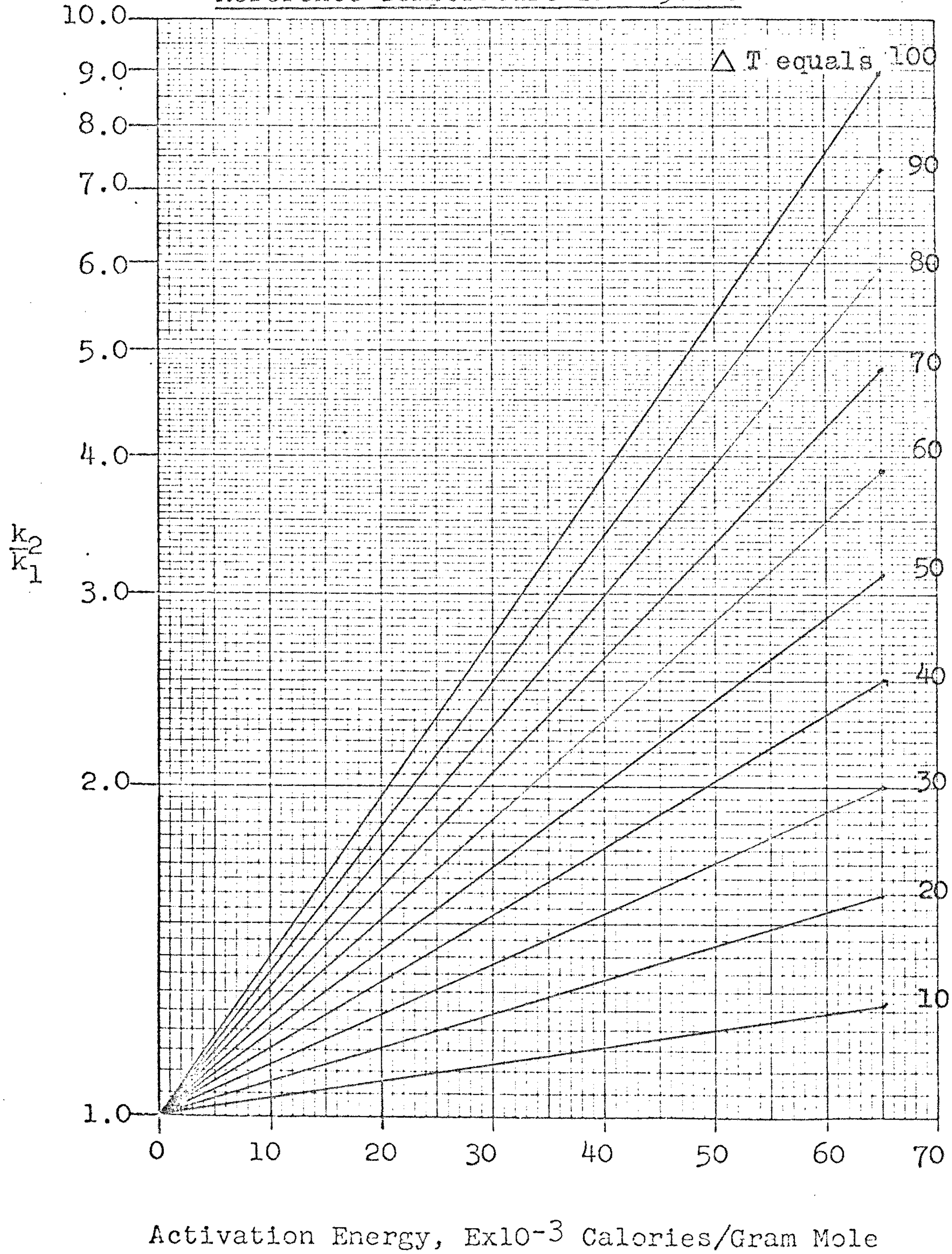
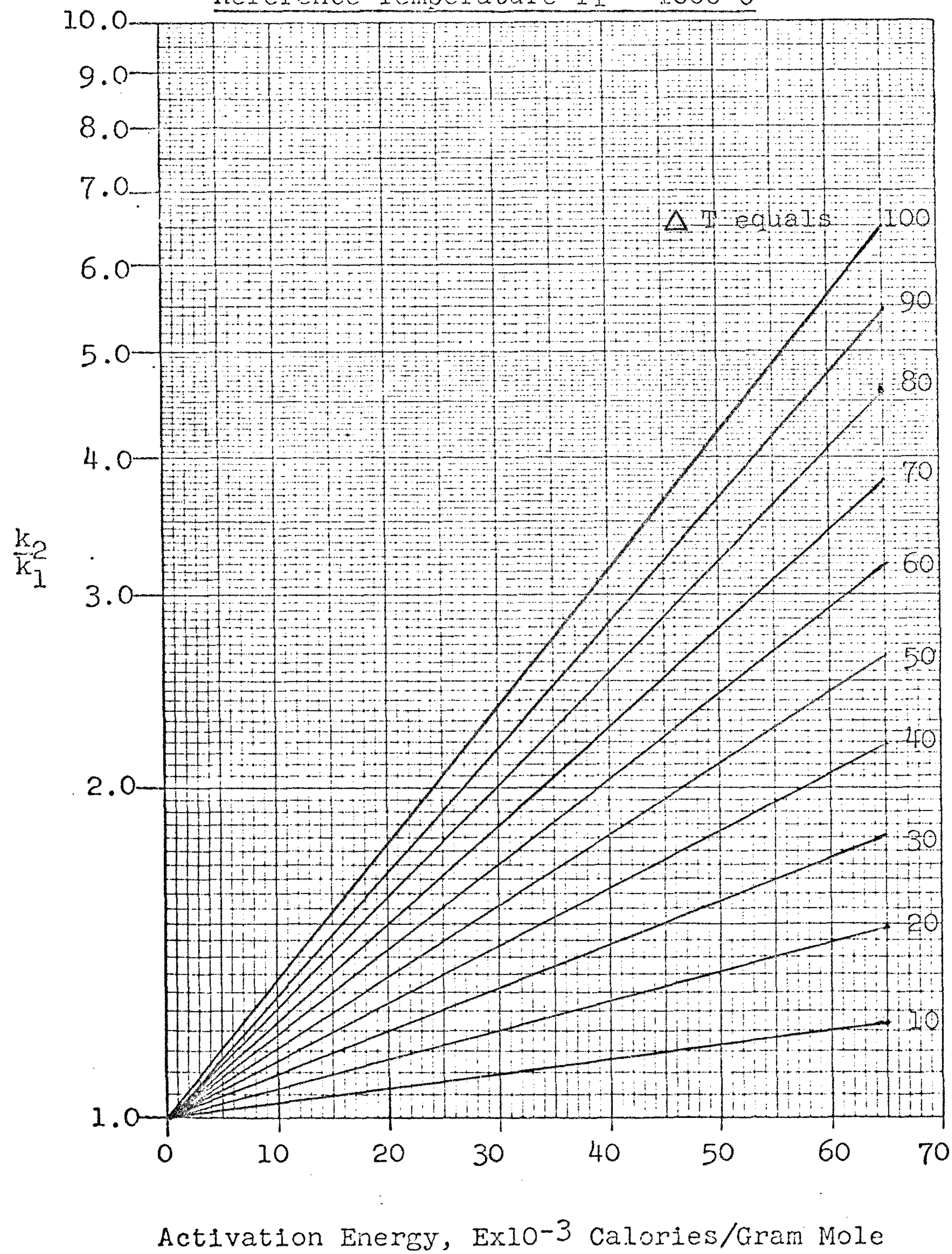


Figure 16

k_2/k_1

Reference Temperature T1 = 1000°C



Program 2

Program for the Calculation of the Ratio K_2/K_1

```
C ARRHENIUS RATE EQUATION PROGRAM FOR THE RATIO K2/K1
C REFERENCE TEMP = -100 TO 1000 DEG C INC. = 50
C ACTIVATION ENERGY = 5000 TO 65000 INC.= 5000
C DELTA TEMP = 1 TO 100 TO LIMIT K2/K1 TO LESS THAN 100
      DIMENSION LL(100),B(100)
      N = 0
      R = 1.98719
C DATA CARD 1
C L = SUBTRACT. CONSTANT FOR TEMP BELOW 0 DEG C
C II,IM,IT = DO LOOP INDEX FOR REF TEMP
C DATA CARD 2
C JI,JM,JT = DO LOOP INDEX FOR ACTIVATION
C ENERGY X 10E-2, EG. 5000 = 50
      READ (2,100) L,II,IM,IT
      READ (2,40) JI,JM,JT
C DO LOOP FOR REF. TEMP
      DO 30 I = II,IM,IT
      N=N+1
      L = L+I
      TC1 = L
C DATA CARD FOR EACH REF TEMP
C KI,KM,KT = DO LOOP INDEX FOR DELTA TEMP
      READ (2,50) KI,KM,KT
C START NEW PAGE
C PRINT TABLE AND HEADINGS AND
C REFERENCE TEMP.
      WRITE (5,90)
      WRITE (5,200)N
      WRITE (5,300) L
      L = L-I
C DO LOOP FOR ACT. ENERGY
      DO 15 K = KI,KM,KT
      LL(K) =K
   15 CONTINUE
C PRINT DELTA T HEADING
      WRITE (5,60)
      WRITE (5,70)    (LL(K),K=KI,KM,KT)
C CALC. K2/K1 FOR EACH DELTA T
      DO 20 J= JI,JM,JT
      EJ = J
      E = EJ * 100.
      DO 10 K = KI,KM,KT
```

```
      TC2 = TC1 + K
      TA1 = TC1 + 273.16
      TA2 = TC2 + 273.16
      ARH = EXP ((-E/R)*((1.0/TA2)-(1.0/TA1)))
      B(K) = ARH
   10 CONTINUE
C PRINT ACT. ENERGY AND K2/K1 FOR EACH DELTA T.
      WRITE (5,80) J,(B(K),K=KI,KM,KT)
   20 CONTINUE
   30 CONTINUE
      WRITE (5,90)
   40 FORMAT (3I3)
   50 FORMAT (3I3)
   60 FORMAT (1H+,49X,'K2/K1 FOR DELTA TEMPERATURE IN DEG
     1C EQUAL TO'//)
   70 FORMAT (1H+,'ACT ENERGY *',8X,10(5X,I3,2X)///)
   80 FORMAT (1H+,2X,I3,'00',13X,10(3X,F7.3)//)
   90 FORMAT (1H+,'* CALORIES PER GRAM MOLE')
  100 FORMAT (4I4)
  200 FORMAT (1H1///////////42X,'TABLE NO. ',I2,' TABULA
     1TED VALUES OF K2/K1'/////)
  300 FORMAT (1H+,43X,'REFERENCE TEMPERATURE = ',I4,' DE
     1G C'///)
      CALL EXIT
      END
```

TABLE NO. 1 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = -100 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	1	2	3	4	5	6	7	8	9	10
5000	1.087	1.180	1.280	1.388	1.503	1.626	1.758	1.899	2.050	2.210
10000	1.181	1.393	1.640	1.927	2.260	2.646	3.093	3.608	4.203	4.887
15000	1.284	1.645	2.100	2.675	3.398	4.305	5.439	6.855	8.617	10.804
20000	1.396	1.941	2.690	3.714	5.109	7.004	9.566	13.022	17.666	23.886
25000	1.517	2.292	3.446	5.157	7.682	11.394	16.825	24.738	36.218	52.806
30000	1.649	2.706	4.413	7.159	11.551	18.536	29.590	46.994	74.253	116.741
35000	1.793	3.194	5.653	9.939	17.367	30.155	52.041	89.272	152.231	258.085
40000	1.949	3.770	7.240	13.799	26.111	49.057	91.525	169.586	312.098	570.560
45000	2.118	4.451	9.273	19.157	39.259	79.808	160.967	322.155	639.850	*******
50000	2.303	5.254	11.876	26.596	59.026	129.833	283.093	611.982	*******	*******
55000	2.503	6.203	15.211	36.924	88.746	211.214	497.878	*******	*******	*******
60000	2.721	7.322	19.481	51.261	133.430	343.607	875.621	*******	*******	*******
65000	2.958	8.644	24.951	71.166	200.612	558.986	*******	*******	*******	*******

* CALORIES PER GRAM MOLE

TABLE NO. 2 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = -50 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	1	2	3	4	5	6	7	8	9	10
5000	1.051	1.105	1.161	1.219	1.280	1.343	1.409	1.477	1.548	1.621
10000	1.105	1.221	1.348	1.487	1.639	1.804	1.985	2.182	2.396	2.630
15000	1.162	1.350	1.566	1.814	2.098	2.424	2.797	3.223	3.710	4.266
20000	1.222	1.492	1.818	2.212	2.686	3.257	3.941	4.762	5.745	6.919
25000	1.285	1.649	2.112	2.698	3.439	4.375	5.554	7.035	8.894	11.221
30000	1.352	1.823	2.453	3.291	4.403	5.878	7.826	10.393	13.770	18.200
35000	1.422	2.015	2.848	4.013	5.638	7.896	11.027	15.354	21.319	29.518
40000	1.495	2.228	3.308	4.895	7.218	10.608	15.538	22.683	33.006	47.973
45000	1.572	2.462	3.842	5.970	9.241	14.251	21.894	33.509	51.101	77.644
50000	1.653	2.722	4.462	7.281	11.832	19.145	30.850	49.503	79.114	125.928
55000	1.738	3.009	5.181	8.881	15.148	25.720	43.469	73.130	122.484	204.238
60000	1.828	3.326	6.017	10.831	19.394	34.553	61.250	108.034	189.629	331.245
65000	1.923	3.676	6.988	13.210	24.831	46.419	86.304	159.597	293.583	537.231

* CALORIES PER GRAM MOLE

TABLE NO. 3 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 0 DEG C

K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO

ACT ENERGY *	2	4	6	8	10	12	14	16	18	20
5000	1.069	1.142	1.218	1.299	1.384	1.473	1.566	1.664	1.767	1.874
10000	1.143	1.304	1.485	1.689	1.916	2.171	2.455	2.771	3.123	3.514
15000	1.222	1.490	1.811	2.195	2.653	3.199	3.846	4.613	5.519	6.587
20000	1.307	1.701	2.207	2.852	3.673	4.713	6.027	7.690	9.755	12.349
25000	1.397	1.943	2.690	3.707	5.086	6.945	9.443	12.786	17.240	23.150
30000	1.494	2.220	3.280	4.818	7.041	10.234	14.797	21.286	30.468	43.398
35000	1.597	2.535	3.998	6.262	9.748	15.079	23.185	35.436	53.846	81.355
40000	1.708	2.896	4.873	8.139	13.495	22.219	36.328	58.993	95.162	152.510
45000	1.826	3.308	5.940	10.578	18.684	32.739	56.920	98.209	168.180	285.898
50000	1.953	3.778	7.240	13.748	25.867	48.240	89.187	163.494	297.224	535.950
55000	2.088	4.315	8.826	17.867	35.812	71.081	139.743	272.177	525.281	*******
60000	2.233	4.929	10.758	23.221	49.579	104.736	218.959	453.109	928.327	*******
65000	2.387	5.630	13.114	30.179	68.640	154.325	343.078	754.316	*******	*******

* CALORIES PER GRAM MOLE

TABLE NO. 4 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 50 DEG C

K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO

ACT ENERGY *	2	4	6	8	10	12	14	16	18	20
5000	1.049	1.099	1.152	1.206	1.263	1.321	1.381	1.443	1.508	1.574
10000	1.100	1.209	1.328	1.456	1.595	1.746	1.909	2.084	2.274	2.479
15000	1.154	1.330	1.530	1.758	2.015	2.307	2.637	3.009	3.429	3.901
20000	1.211	1.463	1.764	2.122	2.546	3.049	3.644	4.345	5.171	6.141
25000	1.270	1.609	2.033	2.561	3.217	4.030	5.035	6.274	7.798	9.669
30000	1.332	1.770	2.343	3.091	4.064	5.326	6.957	9.059	11.760	15.221
35000	1.398	1.947	2.700	3.730	5.134	7.038	9.612	13.080	17.735	23.962
40000	1.466	2.141	3.112	4.502	6.485	9.301	13.281	18.886	26.745	37.722
45000	1.538	2.355	3.587	5.434	8.193	12.291	18.351	27.269	40.333	59.384
50000	1.614	2.590	4.134	6.559	10.350	16.243	25.355	39.372	60.823	93.496
55000	1.693	2.849	4.764	7.916	13.075	21.465	35.033	56.847	91.722	147.171
60000	1.776	3.134	5.490	9.555	16.517	28.366	48.404	82.078	138.319	231.685
65000	1.863	3.447	6.328	11.532	20.865	37.486	66.880	118.508	208.588	364.732

* CALORIES PER GRAM MOLE

TABLE NO. 5 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 100 DEG C

K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO

ACT ENERGY *	3	6	9	12	15	18	21	24	27	30
5000	1.055	1.112	1.172	1.233	1.297	1.363	1.432	1.502	1.576	1.651
10000	1.113	1.237	1.373	1.522	1.683	1.859	2.051	2.258	2.484	2.727
15000	1.175	1.377	1.610	1.878	2.185	2.536	2.937	3.395	3.915	4.505
20000	1.239	1.532	1.887	2.317	2.835	3.459	4.207	5.103	6.170	7.440
25000	1.308	1.704	2.212	2.858	3.679	4.718	6.026	7.669	9.725	12.288
30000	1.380	1.896	2.592	3.527	4.775	6.434	8.631	11.527	15.328	20.296
35000	1.457	2.110	3.039	4.351	6.196	8.775	12.362	17.325	24.159	33.521
40000	1.537	2.348	3.562	5.368	8.040	11.968	17.706	26.040	38.077	55.363
45000	1.622	2.612	4.175	6.623	10.434	16.322	25.359	39.138	60.014	91.438
50000	1.712	2.906	4.893	8.172	13.540	22.260	36.320	58.825	94.587	151.019
55000	1.806	3.233	5.735	10.082	17.570	30.358	52.019	88.414	149.080	249.422
60000	1.906	3.598	6.722	12.440	22.800	41.403	74.504	132.885	234.965	411.945
65000	2.011	4.003	7.879	15.348	29.587	56.466	106.707	199.726	370.328	680.366

* CALORIES PER GRAM MOLE

TABLE NO. 6 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 150 DEG C

K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO

ACT ENERGY *	3	6	9	12	15	18	21	24	27	30
5000	1.042	1.086	1.131	1.178	1.225	1.274	1.324	1.375	1.428	1.482
10000	1.087	1.180	1.281	1.388	1.502	1.624	1.754	1.893	2.040	2.197
15000	1.133	1.283	1.449	1.635	1.841	2.070	2.324	2.604	2.915	3.257
20000	1.182	1.394	1.641	1.926	2.257	2.639	3.078	3.584	4.164	4.828
25000	1.232	1.515	1.857	2.270	2.767	3.363	4.078	4.931	5.948	7.157
30000	1.285	1.646	2.102	2.674	3.391	4.287	5.402	6.785	8.497	10.610
35000	1.340	1.789	2.379	3.151	4.157	5.464	7.155	9.336	12.139	15.728
40000	1.397	1.944	2.692	3.712	5.096	6.964	9.478	12.846	17.341	23.315
45000	1.457	2.113	3.047	4.374	6.246	8.877	12.555	17.676	24.772	34.561
50000	1.519	2.296	3.449	5.153	7.656	11.314	16.631	24.321	35.387	51.232
55000	1.584	2.495	3.904	6.071	9.385	14.420	22.030	33.464	50.551	75.945
60000	1.652	2.711	4.419	7.153	11.503	18.380	29.182	46.045	72.213	112.578
65000	1.723	2.946	5.001	8.428	14.100	23.427	38.655	63.355	103.157	166.881

* CALORIES PER GRAM MOLE

TABLE NO. 7 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 200 DEG C

K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO

ACT ENERGY *	10	20	30	40	50	60	70	80	90	100
5000	1.116	1.240	1.373	1.513	1.662	1.819	1.984	2.157	2.339	2.528
10000	1.246	1.539	1.885	2.291	2.763	3.309	3.937	4.655	5.472	6.395
15000	1.391	1.909	2.588	3.467	4.593	6.021	7.814	10.046	12.800	16.173
20000	1.553	2.369	3.554	5.248	7.636	10.954	15.506	21.676	29.943	40.900
25000	1.733	2.939	4.880	7.944	12.694	19.928	30.771	46.773	70.046	103.432
30000	1.935	3.647	6.701	12.025	21.101	36.255	61.063	100.924	163.856	261.570
35000	2.160	4.524	9.201	18.202	35.078	65.959	121.174	217.769	383.302	661.483
40000	2.412	5.614	12.634	27.551	58.312	119.997	240.459	469.891	896.641	*******
45000	2.692	6.965	17.348	41.701	96.935	218.307	477.169	*******	*******	*******
50000	3.006	8.641	23.821	63.120	161.139	397.158	946.896	*******	*******	*******
55000	3.355	10.721	32.708	95.540	267.869	722.537	*******	*******	*******	*******
60000	3.746	13.301	44.911	144.612	445.289	*******	*******	*******	*******	*******
65000	4.182	16.503	61.667	218.889	740.223	*******	*******	*******	*******	*******

* CALORIES PER GRAM MOLE

TABLE NO. 8 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 250 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	10	20	30	40	50	60	70	80	90	100
5000	1.094	1.193	1.298	1.407	1.521	1.640	1.763	1.892	2.025	2.163
10000	1.197	1.425	1.684	1.980	2.314	2.690	3.111	3.581	4.103	4.681
15000	1.310	1.701	2.186	2.786	3.520	4.412	5.488	6.778	8.312	10.128
20000	1.434	2.030	2.838	3.921	5.356	7.237	9.682	12.827	16.839	21.914
25000	1.569	2.424	3.684	5.518	8.148	11.871	17.079	24.276	34.112	47.414
30000	1.718	2.893	4.782	7.765	12.395	19.472	30.127	45.943	69.104	102.587
35000	1.880	3.454	6.208	10.926	18.857	31.939	53.144	86.947	139.986	221.960
40000	2.057	4.123	8.058	15.376	28.687	52.387	93.746	164.549	283.577	480.239
45000	2.252	4.922	10.459	21.637	43.641	85.928	165.366	311.411	574.454	*******
50000	2.464	5.876	13.576	30.448	66.391	140.941	291.704	589.347	*******	*******
55000	2.697	7.014	17.622	42.847	101.000	231.176	514.560	*******	*******	*******
60000	2.951	8.373	22.874	60.295	153.650	379.181	907.676	*******	*******	*******
65000	3.230	9.996	29.691	84.848	233.746	621.943	*******	*******	*******	*******

* CALORIES PER GRAM MOLE

TABLE NO. 9 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 300 DEG C

	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
ACT ENERGY *	10	20	30	40	50	60	70	80	90	100
5000	1.078	1.159	1.244	1.331	1.422	1.515	1.612	1.712	1.814	1.919
10000	1.162	1.344	1.547	1.773	2.022	2.297	2.600	2.931	3.292	3.684
15000	1.253	1.559	1.925	2.361	2.876	3.483	4.192	5.018	5.973	7.073
20000	1.351	1.807	2.394	3.144	4.091	5.280	6.760	8.591	10.838	13.579
25000	1.457	2.096	2.979	4.186	5.819	8.004	10.901	14.708	19.665	26.066
30000	1.570	2.430	3.706	5.574	8.276	12.133	17.579	25.181	35.681	50.039
35000	1.693	2.818	4.610	7.423	11.770	18.393	28.346	43.110	64.740	96.056
40000	1.826	3.267	5.735	9.885	16.740	27.882	45.708	73.807	117.467	184.393
45000	1.968	3.789	7.135	13.163	23.809	42.266	73.705	126.360	213.137	353.967
50000	2.122	4.393	8.876	17.527	33.862	64.071	118.850	216.333	386.722	679.487
55000	2.288	5.094	11.043	23.340	48.159	97.124	191.646	370.370	701.679	*******
60000	2.467	5.907	13.737	31.079	68.494	147.230	309.030	634.087	*******	*******
65000	2.660	6.849	17.089	41.385	97.415	223.184	498.311	*******	*******	*******

* CALORIES PER GRAM MOLE

TABLE NO. 10 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 350 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO 10	20	30	40	50	60	70	80	90	100
5000	1.065	1.133	1.203	1.275	1.349	1.425	1.503	1.583	1.664	1.747
10000	1.136	1.285	1.449	1.627	1.821	2.032	2.260	2.506	2.770	3.054
15000	1.210	1.457	1.744	2.076	2.458	2.897	3.398	3.967	4.611	5.338
20000	1.290	1.652	2.099	2.648	3.318	4.130	5.109	6.280	7.676	9.331
25000	1.375	1.873	2.527	3.379	4.479	5.889	7.681	9.943	12.778	16.308
30000	1.466	2.124	3.042	4.311	6.046	8.395	11.547	15.740	21.270	28.503
35000	1.562	2.408	3.662	5.500	8.160	11.969	17.361	24.918	35.404	49.817
40000	1.665	2.730	4.408	7.016	11.014	17.063	26.102	39.448	58.932	87.069
45000	1.775	3.095	5.307	8.951	14.866	24.326	39.242	62.450	98.096	152.176
50000	1.892	3.509	6.388	11.420	20.066	34.680	58.998	98.864	163.285	265.968
55000	2.016	3.979	7.690	14.569	27.084	49.441	88.700	156.510	271.795	464.850
60000	2.149	4.511	9.257	18.587	36.556	70.485	133.355	247.769	452.415	812.449
65000	2.291	5.115	11.143	23.713	49.341	100.487	200.491	392.240	753.064	*******

* CALORIES PER GRAM MOLE

TABLE NO. 11 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 400 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	10	20	30	40	50	60	70	80	90	100
5000	1.056	1.113	1.172	1.233	1.294	1.357	1.422	1.487	1.553	1.621
10000	1.115	1.240	1.375	1.520	1.676	1.843	2.022	2.212	2.414	2.629
15000	1.178	1.382	1.613	1.875	2.171	2.503	2.875	3.290	3.752	4.264
20000	1.244	1.539	1.892	2.313	2.811	3.399	4.088	4.894	5.831	6.915
25000	1.314	1.714	2.219	2.852	3.640	4.615	5.814	7.279	9.061	11.214
30000	1.388	1.909	2.603	3.517	4.714	6.267	8.268	10.828	14.080	18.185
35000	1.466	2.127	3.053	4.338	6.104	8.509	11.757	16.105	21.880	29.491
40000	1.549	2.369	3.581	5.350	7.904	11.555	16.719	23.955	34.000	47.823
45000	1.636	2.639	4.200	6.598	10.235	15.689	23.774	35.630	52.835	77.553
50000	1.728	2.940	4.926	8.137	13.254	21.304	33.807	52.996	82.103	125.764
55000	1.825	3.275	5.778	10.035	17.163	28.927	48.075	78.826	127.584	203.944
60000	1.928	3.647	6.777	12.375	22.224	39.278	68.363	117.246	198.259	330.726
65000	2.036	4.063	7.949	15.262	28.778	53.333	97.212	174.390	308.083	536.321

* CALORIES PER GRAM MOLE

TABLE NO. 12 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 450 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	10	20	30	40	50	60	70	80	90	100
5000	1.048	1.098	1.148	1.200	1.252	1.305	1.359	1.414	1.469	1.526
10000	1.099	1.205	1.319	1.440	1.568	1.704	1.848	1.999	2.160	2.328
15000	1.153	1.324	1.515	1.728	1.964	2.224	2.512	2.828	3.174	3.553
20000	1.209	1.454	1.740	2.073	2.459	2.904	3.415	3.999	4.666	5.423
25000	1.267	1.597	1.999	2.488	3.080	3.791	4.642	5.656	6.858	8.276
30000	1.329	1.753	2.296	2.986	3.857	4.949	6.311	7.999	10.079	12.630
35000	1.394	1.926	2.638	3.584	4.831	6.461	8.580	11.313	14.814	19.274
40000	1.461	2.115	3.030	4.301	6.050	8.435	11.664	15.998	21.774	29.413
45000	1.532	2.322	3.480	5.161	7.576	11.012	15.856	22.625	32.002	44.885
50000	1.607	2.550	3.998	6.194	9.488	14.376	21.556	31.997	47.035	68.498
55000	1.685	2.801	4.592	7.433	11.882	18.768	29.304	45.250	69.130	104.531
60000	1.767	3.076	5.275	8.920	14.881	24.501	39.837	63.993	101.604	159.519
65000	1.853	3.377	6.059	10.705	18.636	31.985	54.156	90.499	149.333	243.434

* CALCRIES PER GRAM MOLE

TABLE NO. 13 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 500 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	10	20	30	40	50	60	70	80	90	100
5000	1.042	1.085	1.129	1.173	1.218	1.264	1.310	1.356	1.403	1.451
10000	1.086	1.178	1.275	1.377	1.484	1.597	1.716	1.841	1.971	2.107
15000	1.132	1.279	1.440	1.616	1.809	2.019	2.249	2.497	2.767	3.059
20000	1.180	1.388	1.626	1.897	2.204	2.553	2.946	3.389	3.885	4.440
25000	1.230	1.507	1.836	2.226	2.686	3.227	3.860	4.598	5.455	6.446
30000	1.283	1.636	2.073	2.613	3.274	4.080	5.058	6.239	7.659	9.358
35000	1.337	1.776	2.341	3.066	3.989	5.157	6.627	8.466	10.753	13.584
40000	1.394	1.927	2.644	3.599	4.861	6.520	8.683	11.487	15.098	19.720
45000	1.453	2.092	2.986	4.223	5.924	8.242	11.377	15.586	21.197	28.627
50000	1.515	2.271	3.372	4.957	7.219	10.418	14.906	21.148	29.761	41.557
55000	1.579	2.466	3.808	5.817	8.796	13.170	19.530	28.694	41.785	60.326
60000	1.646	2.677	4.300	6.827	10.719	16.648	25.588	38.934	58.666	87.574
65000	1.716	2.906	4.856	8.013	13.062	21.045	33.525	52.827	82.367	127.127

* CALORIES PER GRAM MOLE

TABLE NO. 14 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 550 DEG C

K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO

ACT ENERGY *	10	20	30	40	50	60	70	80	90	100
5000	1.037	1.075	1.113	1.152	1.191	1.230	1.270	1.310	1.351	1.392
10000	1.076	1.156	1.239	1.327	1.419	1.514	1.614	1.718	1.826	1.939
15000	1.116	1.242	1.380	1.529	1.690	1.864	2.051	2.252	2.468	2.700
20000	1.158	1.336	1.537	1.762	2.014	2.294	2.607	2.953	3.336	3.760
25000	1.201	1.436	1.711	2.030	2.399	2.824	3.312	3.871	4.510	5.235
30000	1.246	1.545	1.905	2.339	2.858	3.476	4.209	5.075	6.095	7.291
35000	1.292	1.661	2.122	2.695	3.404	4.278	5.349	6.654	8.238	10.152
40000	1.341	1.786	2.362	3.105	4.056	5.266	6.797	8.723	11.134	14.138
45000	1.391	1.920	2.630	3.578	4.832	6.481	8.636	11.436	15.049	19.687
50000	1.443	2.064	2.929	4.122	5.756	7.977	10.974	14.992	20.340	27.414
55000	1.497	2.220	3.261	4.750	6.857	9.818	13.945	19.653	27.491	38.175
60000	1.553	2.387	3.632	5.472	8.169	12.084	17.720	25.765	37.155	53.159
65000	1.611	2.566	4.044	6.305	9.732	14.874	22.517	33.776	50.218	74.025

* CALORIES PER GRAM MOLE

TABLE NO. 15 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 600 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	10	20	30	40	50	60	70	80	90	100
5000	1.033	1.066	1.100	1.134	1.168	1.203	1.238	1.273	1.309	1.344
10000	1.067	1.137	1.210	1.287	1.366	1.448	1.533	1.622	1.713	1.807
15000	1.102	1.213	1.332	1.460	1.597	1.743	1.899	2.065	2.242	2.431
20000	1.139	1.294	1.466	1.656	1.866	2.098	2.352	2.631	2.936	3.268
25000	1.177	1.380	1.613	1.879	2.182	2.525	2.913	3.351	3.843	4.395
30000	1.216	1.472	1.775	2.132	2.550	3.039	3.608	4.268	5.030	5.910
35000	1.256	1.570	1.954	2.419	2.981	3.658	4.468	5.435	6.585	7.946
40000	1.298	1.675	2.150	2.745	3.485	4.402	5.534	6.923	8.620	10.685
45000	1.341	1.787	2.366	3.114	4.074	5.299	6.853	8.817	11.284	14.367
50000	1.385	1.906	2.604	3.533	4.762	6.377	8.488	11.229	14.770	19.319
55000	1.431	2.033	2.865	4.008	5.566	7.676	10.512	14.302	19.335	25.977
60000	1.479	2.169	3.153	4.548	6.507	9.238	13.019	18.216	25.309	34.929
65000	1.528	2.313	3.470	5.160	7.606	11.119	16.123	23.200	33.130	46.966

* CALORIES PER GRAM MOLE

TABLE NO. 16 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 650 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	10	20	30	40	50	60	70	80	90	100
5000	1.029	1.059	1.089	1.119	1.150	1.180	1.211	1.242	1.273	1.305
10000	1.060	1.122	1.187	1.254	1.323	1.394	1.468	1.544	1.622	1.703
15000	1.091	1.189	1.293	1.404	1.522	1.647	1.779	1.919	2.067	2.223
20000	1.123	1.260	1.409	1.572	1.750	1.945	2.156	2.385	2.633	2.902
25000	1.157	1.335	1.535	1.761	2.014	2.297	2.613	2.964	3.355	3.788
30000	1.191	1.414	1.673	1.972	2.316	2.712	3.166	3.684	4.274	4.944
35000	1.226	1.498	1.823	2.208	2.665	3.203	3.837	4.579	5.445	6.453
40000	1.263	1.587	1.986	2.473	3.065	3.783	4.649	5.690	6.937	8.424
45000	1.300	1.682	2.164	2.769	3.526	4.468	5.634	7.072	8.837	10.995
50000	1.339	1.782	2.358	3.101	4.056	5.276	6.827	8.789	11.258	14.351
55000	1.378	1.888	2.569	3.473	4.666	6.231	8.274	10.923	14.342	18.732
60000	1.419	2.000	2.799	3.889	5.367	7.359	10.026	13.575	18.271	24.449
65000	1.461	2.119	3.050	4.355	6.174	8.691	12.150	16.871	23.277	31.913

* CALORIES PER GRAM MOLE

TABLE NO. 17 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 700 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	10	20	30	40	50	60	70	80	90	100
5000	1.026	1.053	1.080	1.107	1.134	1.162	1.189	1.217	1.244	1.272
10000	1.054	1.109	1.167	1.226	1.287	1.350	1.414	1.481	1.549	1.619
15000	1.082	1.169	1.261	1.358	1.460	1.569	1.682	1.802	1.928	2.060
20000	1.110	1.231	1.362	1.504	1.657	1.823	2.001	2.193	2.400	2.621
25000	1.140	1.297	1.471	1.665	1.880	2.118	2.380	2.669	2.987	3.335
30000	1.170	1.366	1.590	1.844	2.134	2.461	2.832	3.249	3.718	4.244
35000	1.202	1.439	1.718	2.043	2.421	2.860	3.368	3.954	4.627	5.400
40000	1.234	1.516	1.856	2.262	2.747	3.324	4.006	4.812	5.760	6.871
45000	1.267	1.597	2.005	2.506	3.117	3.862	4.765	5.856	7.169	8.743
50000	1.300	1.683	2.166	2.775	3.537	4.488	5.668	7.127	8.923	11.125
55000	1.335	1.773	2.340	3.073	4.014	5.215	6.742	8.674	11.107	14.156
60000	1.371	1.867	2.529	3.403	4.554	6.060	8.020	10.557	13.824	18.013
65000	1.407	1.967	2.732	3.769	5.168	7.042	9.539	12.848	17.207	22.920

* CALORIES PER GRAM MOLE

TABLE NO. 18 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 750 DEG C

K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO

ACT ENERGY *	10	20	30	40	50	60	70	80	90	100
5000	1.024	1.048	1.072	1.096	1.121	1.145	1.170	1.195	1.219	1.244
10000	1.048	1.098	1.150	1.203	1.257	1.313	1.370	1.428	1.488	1.549
15000	1.074	1.151	1.233	1.319	1.410	1.504	1.603	1.707	1.815	1.928
20000	1.099	1.207	1.323	1.447	1.581	1.724	1.877	2.040	2.215	2.400
25000	1.126	1.265	1.419	1.588	1.773	1.976	2.197	2.439	2.702	2.988
30000	1.153	1.326	1.522	1.742	1.988	2.264	2.572	2.915	3.296	3.719
35000	1.181	1.391	1.632	1.911	2.230	2.594	3.011	3.484	4.021	4.630
40000	1.209	1.458	1.751	2.096	2.500	2.973	3.524	4.164	4.906	5.763
45000	1.238	1.528	1.878	2.299	2.804	3.407	4.125	4.977	5.986	7.174
50000	1.268	1.602	2.014	2.522	3.144	3.904	4.829	5.949	7.302	8.930
55000	1.299	1.679	2.160	2.766	3.526	4.474	5.653	7.111	8.909	11.116
60000	1.330	1.760	2.317	3.035	3.954	5.127	6.617	8.499	10.868	13.837
65000	1.362	1.845	2.485	3.329	4.434	5.876	7.745	10.159	13.259	17.224

* CALORIES PER GRAM MOLE

TABLE NO. 19 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 800 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	10	20	30	40	50	60	70	80	90	100
5000	1.021	1.043	1.065	1.087	1.110	1.132	1.154	1.176	1.198	1.221
10000	1.044	1.089	1.136	1.183	1.232	1.281	1.332	1.384	1.437	1.491
15000	1.067	1.137	1.210	1.287	1.367	1.451	1.538	1.628	1.723	1.821
20000	1.090	1.187	1.290	1.400	1.518	1.643	1.775	1.916	2.066	2.224
25000	1.114	1.239	1.375	1.523	1.685	1.860	2.049	2.255	2.477	2.716
30000	1.138	1.293	1.466	1.657	1.870	2.106	2.366	2.653	2.969	3.317
35000	1.163	1.350	1.562	1.803	2.076	2.384	2.731	3.122	3.560	4.051
40000	1.189	1.409	1.665	1.962	2.304	2.699	3.153	3.673	4.268	4.947
45000	1.215	1.471	1.775	2.134	2.558	3.056	3.640	4.322	5.117	6.041
50000	1.241	1.535	1.891	2.322	2.839	3.460	4.202	5.086	6.135	7.378
55000	1.268	1.602	2.016	2.526	3.152	3.918	4.851	5.984	7.356	9.010
60000	1.296	1.673	2.149	2.748	3.499	4.435	5.600	7.041	8.819	11.003
65000	1.324	1.746	2.290	2.989	3.884	5.022	6.464	8.285	10.573	13.437

* CALORIES PER GRAM MOLE

TABLE NO. 20 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 850 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	10	20	30	40	50	60	70	80	90	100
5000	1.019	1.039	1.060	1.080	1.100	1.120	1.140	1.160	1.180	1.200
10000	1.040	1.081	1.123	1.166	1.210	1.255	1.300	1.347	1.394	1.442
15000	1.061	1.124	1.191	1.260	1.331	1.406	1.483	1.563	1.646	1.732
20000	1.082	1.169	1.262	1.360	1.465	1.575	1.691	1.814	1.944	2.080
25000	1.103	1.216	1.338	1.469	1.611	1.764	1.929	2.105	2.295	2.498
30000	1.125	1.265	1.418	1.587	1.773	1.977	2.200	2.444	2.710	3.000
35000	1.148	1.315	1.503	1.714	1.951	2.214	2.509	2.836	3.200	3.604
40000	1.171	1.368	1.593	1.852	2.146	2.481	2.861	3.292	3.779	4.328
45000	1.194	1.422	1.689	2.000	2.361	2.779	3.263	3.821	4.462	5.198
50000	1.218	1.479	1.791	2.160	2.598	3.114	3.722	4.435	5.269	6.243
55000	1.242	1.538	1.898	2.333	2.858	3.489	4.244	5.147	6.222	7.498
60000	1.267	1.600	2.012	2.520	3.144	3.908	4.841	5.974	7.347	9.005
65000	1.293	1.664	2.133	2.722	3.459	4.379	5.521	6.933	8.675	10.815

* CALORIES PER GRAM MOLE

TABLE NO. 21 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 900 DEG C

K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO

ACT ENERGY *	10	20	30	40	50	60	70	80	90	100
5000	1.018	1.036	1.054	1.073	1.091	1.109	1.128	1.146	1.165	1.183
10000	1.036	1.074	1.112	1.151	1.191	1.232	1.273	1.314	1.357	1.400
15000	1.055	1.113	1.174	1.236	1.300	1.367	1.436	1.507	1.581	1.657
20000	1.075	1.154	1.238	1.326	1.420	1.518	1.621	1.729	1.842	1.961
25000	1.094	1.196	1.306	1.424	1.550	1.685	1.829	1.982	2.146	2.321
30000	1.114	1.240	1.378	1.528	1.692	1.870	2.063	2.273	2.501	2.747
35000	1.135	1.286	1.454	1.640	1.847	2.076	2.328	2.607	2.914	3.251
40000	1.156	1.333	1.533	1.760	2.016	2.304	2.627	2.990	3.395	3.848
45000	1.177	1.382	1.618	1.889	2.201	2.557	2.965	3.428	3.956	4.554
50000	1.198	1.432	1.707	2.028	2.403	2.839	3.345	3.932	4.609	5.390
55000	1.220	1.485	1.800	2.176	2.623	3.151	3.775	4.509	5.370	6.379
60000	1.243	1.539	1.899	2.336	2.863	3.498	4.259	5.170	6.257	7.549
65000	1.265	1.595	2.004	2.507	3.125	3.882	4.806	5.929	7.290	8.934

* CALORIES PER GRAM MOLE

TABLE NO. 22 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 950 DEG C

K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO

ACT ENERGY *	10	20	30	40	50	60	70	80	90	100
5000	1.016	1.033	1.050	1.067	1.084	1.100	1.117	1.134	1.151	1.168
10000	1.033	1.068	1.103	1.139	1.175	1.212	1.249	1.287	1.325	1.364
15000	1.051	1.104	1.159	1.215	1.274	1.334	1.396	1.460	1.526	1.594
20000	1.069	1.141	1.217	1.297	1.381	1.469	1.561	1.657	1.757	1.862
25000	1.086	1.179	1.279	1.385	1.497	1.617	1.745	1.880	2.023	2.175
30000	1.105	1.219	1.343	1.478	1.623	1.780	1.950	2.133	2.330	2.541
35000	1.123	1.260	1.411	1.577	1.760	1.960	2.180	2.420	2.682	2.969
40000	1.142	1.303	1.482	1.683	1.908	2.158	2.437	2.746	3.089	3.468
45000	1.161	1.346	1.557	1.797	2.069	2.376	2.724	3.115	3.556	4.051
50000	1.181	1.392	1.636	1.918	2.243	2.616	3.045	3.535	4.095	4.733
55000	1.201	1.439	1.718	2.047	2.431	2.880	3.403	4.011	4.715	5.529
60000	1.221	1.487	1.805	2.185	2.636	3.171	3.804	4.551	5.429	6.459
65000	1.242	1.537	1.896	2.332	2.858	3.491	4.252	5.163	6.251	7.546

* CALORIES PER GRAM MOLE

TABLE NO. 23 TABULATED VALUES OF K2/K1

REFERENCE TEMPERATURE = 1000 DEG C

ACT ENERGY *	K2/K1 FOR DELTA TEMPERATURE IN DEG C EQUAL TO									
	10	20	30	40	50	60	70	80	90	100
5000	1.015	1.031	1.046	1.062	1.077	1.093	1.108	1.123	1.139	1.154
10000	1.031	1.063	1.095	1.127	1.161	1.194	1.228	1.263	1.298	1.333
15000	1.047	1.096	1.146	1.197	1.251	1.305	1.362	1.419	1.479	1.539
20000	1.063	1.130	1.199	1.272	1.348	1.427	1.509	1.595	1.685	1.778
25000	1.080	1.165	1.255	1.351	1.452	1.560	1.673	1.793	1.920	2.053
30000	1.096	1.201	1.313	1.435	1.565	1.705	1.855	2.015	2.187	2.371
35000	1.113	1.238	1.375	1.524	1.686	1.863	2.056	2.265	2.492	2.738
40000	1.131	1.277	1.439	1.618	1.817	2.037	2.279	2.546	2.840	3.162
45000	1.148	1.316	1.506	1.719	1.958	2.226	2.526	2.862	3.235	3.652
50000	1.166	1.357	1.576	1.825	2.110	2.433	2.800	3.216	3.686	4.217
55000	1.184	1.399	1.649	1.939	2.273	2.660	3.104	3.615	4.200	4.870
60000	1.203	1.443	1.726	2.059	2.450	2.907	3.441	4.063	4.786	5.474
65000	1.221	1.487	1.806	2.187	2.640	3.178	3.815	4.567	5.453	6.494

* CALORIES PER GRAM MOLE

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