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AUTHOR	Hanock, John J.
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ABSTRACT

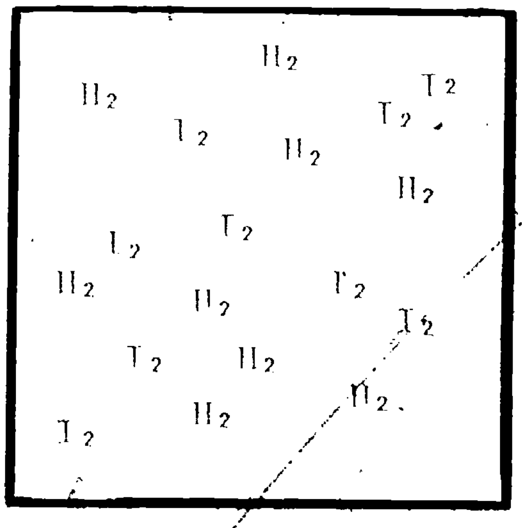
Presented are the teacher's guide and student materials for one of a series of self-instructional, computer-based learning modules for an introductory, undergraduate chemistry course. The student module for this introductory unit on chemical equilibrium includes objectives, prerequisites, pretest, instructions for executing the computer program, and problems. Included in the teacher's guide are implementation instructions, software, sample run, and listings of the computer program in both BASIC and FORTRAN. (BT)

CHEMICAL EQUILIBRIUM

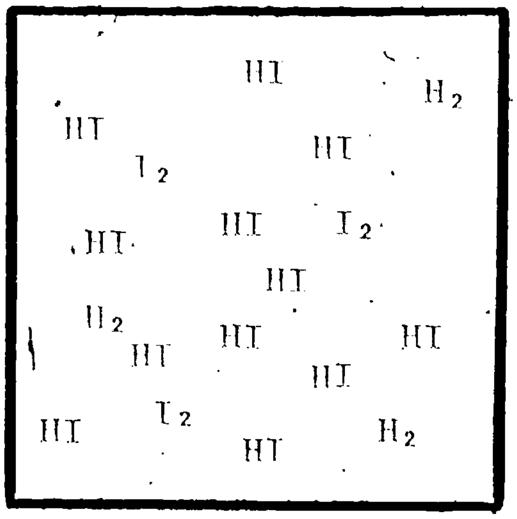
UNIT 1. INTRODUCTION TO CHEMICAL EQUILIBRIUM

JOHN J. MANOCK
WESTERN CAROLINA UNIVERSITY

A COMPUTER-ENRICHED MODULE
FOR INTRODUCTORY CHEMISTRY



In the beginning



at equilibrium

Mary L. Charles
NSF

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OBJECTIVES

When you finish this module you will be able to

1. understand the meaning of chemical equilibrium.
2. write an equilibrium expression for any chemical reaction.
3. predict the direction that a reaction will proceed from the magnitude of the equilibrium constant.
4. explain the significance of the magnitude of an equilibrium constant in terms of the completeness of a reaction.
5. know how to write the equilibrium expression for reactions involving pure liquids or pure solids.

PREREQUISITES

Before you start this module you should understand

1. the mole concept.
2. stoichiometry of chemical reactions.

PRE-TEST

The purpose of this self-test is for you to decide whether or not you have mastered the prerequisites. If you miss more than one question from the following set, it is suggested that you review the material in the modules on mole concept and stoichiometry.

1. Given the following balanced chemical equation:

   $$2\ NaOH + H_2SO_4 = Na_2SO_4 + 2\ H_2O$$

   Assuming the reaction goes to completion,

   a) calculate the number of moles of Na_2SO_4 formed when 1.5 moles of NaOH react with an excess amount of H_2SO_4.

   b) calculate the number of moles of H_2SO_4 required to react with 55.0 grams of NaOH.

2. In the reaction:

   $$2\ H_2 + O_2 \rightleftharpoons 2\ H_2O$$

   25.0 grams of H_2 are mixed with 25.0 grams of O_2.

   a) Determine which reactant is in excess.

   b) Determine the theoretical yield of H_2O.

   c) How many moles of the reactant in excess will remain after the reaction has gone to completion?

Answers to pre-test:

1. a) 0.75 moles Na_2SO_4 b) 0.688 moles H_2SO_4
2. a) H_2 in excess b) 28.1 grams H_2O c) 10.9 moles H_2

INTRODUCTION

To illustrate the concept of chemical equilibrium a computer program, referred to in this discussion as EQSIM, has been developed to simulate a system achieving an equilibrium state. At this point you should use EQSIM and return to this study guide after you have seen the simulated illustrations of the chemical system.

Execute the computer program, EQSIM.

Now, using the illustrations simulated by EQSIM attempt to answer the following questions.

1) How do the illustrations differ?

Obviously, the number of A, B, and C molecules change as the time changes. However, in the case of the last two illustrations in each sequence the number of A, B, and C molecules does not change. Although the positions of the molecules change indicating that the system is in a state of dynamic equilibrium, the numbers of the individual molecules do not change.

2) How are the illustrations in the last two sequences similar?

In both cases the law of conservation of mass is shown. For each A molecule which decomposes, corresponding B and C molecules are formed. In addition, note that regardless whether the reaction is initially started from the left (all A) or from the right (all B and C), the final equilibrium state is the same. In all cases where a chemical reaction occurs the system will ultimately achieve an equilibrium state where the measured concentrations of the products and reactants do not change. At this point the system is at equilibrium.

Having seen that when a system is at equilibrium the concentrations of the products and reactants do not change, now consider quantitatively a chemical system and determine whether or not there is a mathematical relationship among the equilibrium concentrations which is unique to that system. Use the computer program KEQ and then return to this study guide.

Execute the computer program KEQ.

You have observed from the simulated experimental data that the equilibrium concentrations of the products divided by those of the reactants (both expressed in moles/liter) raised to the respective coefficients of the balanced chemical equation are equal to a constant value. This constant is referred to as the equilibrium constant for that particular reaction. For a general reaction:

$$aA + bB \rightleftharpoons cC + dD$$

$$K = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

where K is the equilibrium constant and [A], [B], [C], and [D] are the equilibrium concentrations, expressed in moles/liter. Obviously, a constant would also be obtained if the concentrations of the reactants were divided by the concentrations of the products. However, it is chosen by convention to write the products over the reactants. For example, in the case of the reaction

$$2\ SO_2 + O_2 \rightleftharpoons 2\ SO_3$$

the equilibrium constant is written as

$$K = \frac{[SO_3]^2}{[SO_2]^2[O_2]}$$

However, in the case of the reverse reaction

$$2\ SO_3 \rightleftharpoons 2\ SO_2 + O_2$$

the equilibrium constant is written as

$$K' = \frac{[SO_2]^2[O_2]}{[SO_3]^2} = \frac{1}{K}$$

again following the convention of the concentrations of the products divided by the concentrations of the reactants. This is an important fact to remember.

Problem 1. Write the equilibrium constant expressions for the following reactions:

a) $N_2(g) + 3\ H_2(g) \rightleftharpoons 2\ NH_3(g)$ K = ?

b) $SO_2(g) + NO_2(g) \rightleftharpoons SO_3(g) + NO(g)$ K = ?

c) $2\ NO(g) + O_2(g) \rightleftharpoons 2\ NO_2(g)$ K = ?

A large amount of information can be obtained from the equilibrium constant. Since the equilibrium constant is equal to the product concentrations divided by the reactant equilibrium concentrations, you can use the magnitude of the equilibrium constant to predict the extent of the reaction.

For example, consider the reaction

$$2\ NO(g) + O_2(g) \rightleftharpoons 2\ NO_2(g)\ .$$

The value of the equilibrium constant is 71 at 460°C. Thus, in this case $[NO_2]^2$ is much greater than $[O_2][NO]^2$, indicating that the reaction exists at equilibrium primarily as $NO_2(g)$. This has all been deduced by simply considering the magnitude of the equilibrium constant. For the reaction:

$$2\ HI(g) \rightleftharpoons H_2(g) + I_2(g)$$

$$K = 1.6 \times 10^{-2} = \frac{[H_2][I_2]}{[HI]^2}$$

thus indicating that in the case of this reaction, the system consists primarily of HI at equilibrium. In general, you should be able to look at the magnitude of K and estimate whether the reaction favors the reactants or products.

Problem 2. For the following reactions use the magnitude of the equilibrium constant to estimate whether the system at equilibrium will consist primarily of products or reactants.

a) $N_2(g) + O_2(g) \rightleftharpoons 2\,NO(g)$ $\quad K = 0.10$

b) $SO_2(g) + NO_2(g) \rightleftharpoons SO_3(g) + NO(g)$ $\quad K = 9.0$

c) $CO(g) + \frac{1}{2}O_2(g) \rightleftharpoons CO_2(g)$ $\quad K = 1 \times 10^4$

In addition to estimating the extent of a given reaction, the equilibrium constant can also be useful in determining the direction a reaction proceeds from a given set of initial concentrations. For example, consider the reaction

$$2\,NO(g) + O_2(g) \rightleftharpoons 2\,NO_2(g) \qquad K = 71 .$$

Suppose you were to mix 3 moles $NO(g)$, 2 moles $O_2(g)$, and 5 moles $NO_2(g)$ in a 2-liter flask. In which direction would the reaction proceed to obtain equilibrium? The first step needed to answer this question is to calculate the reaction quotient which is defined as the concentrations of the products divided by the concentrations of the reactants raised to their respective coefficients. Note: This quantity does not equal the equilibrium constant unless the concentrations are the equilibrium concentrations.

In the example cited above, the reaction quotient, Q, is equal to:

$$Q = \frac{[NO_2]^2}{[NO]^2[O_2]} = \frac{(5/2)^2}{(3/2)^2(2/2)} = 2.78 .$$

Therefore, for this set of initial conditions, the reaction quotient, Q, is less than the equilibrium constant, K. How will the reaction proceed in order that the reaction quotient becomes equal to the equilibrium constant?

In this example the concentration of the product must increase and the concentrations of the reactants decrease in order for Q to become equal to K. Thus, the reaction must proceed to the right to attain equilibrium. This example shows that the equilibrium constant can be used to determine the direction a reaction will proceed from a given set of initial concentrations.

Problem 3. For the system $N_2O_4(g) \rightleftharpoons 2NO_2(g)$, $K = 0.90$. Predict the direction in which each of the following systems will move to achieve equilibrium.

a) $[NO_2] = 0.50$ moles/liter, $[N_2O_4] = 0.50$ moles/liter.

b) 2.0 moles of NO_2 and 1.0 moles of N_2O_4 in a 3.0 liter flask.

Problem 4. For the system $2HI(g) \rightleftharpoons H_2(g) + I_2(g)$, $K = 0.016$. Predict the direction in which each of the following systems will move to achieve equilibrium.

a) 2.0 moles of HI, 1.0 moles of I_2, and 1.0 moles of H_2 in a 5.0 liter flask.

b) 0.01 moles of HI, 20.0 moles of I_2, and 0.00 moles of H_2 in a 2.0 liter flask.

We have discovered that for a general gaseous reaction

$$aA + bB \rightleftharpoons cC + dD$$

the expression

$$K = \frac{[C]^c[D]^d}{[A]^a[B]^b},$$

where [A], [B], [C], and [D] are the equilibrium concentrations expressed in moles per liter, is a constant unique for that reaction at a given temperature. This is true for any reaction where all the reactants and products are gases.

However, if any of the components in the reaction are pure liquids or pure solids, the concentration, moles/liter, is proportional to the density of that substance and will remain constant at a constant temperature. Therefore, in the reactions which involve pure solids or pure liquids, the concentrations, moles/liter, of the liquids and solids are incorporated into the value of the equilibrium constant. It is imperative that the phases, or physical states, of the reactants and products be written as part of the chemical equation. We will designate g, l, and s to represent gas, liquid, and solid, respectively.

Consider the reaction

$$CaCO_3(s) \rightleftharpoons CaO(s) + CO_2(g) .$$

For this reaction, the equilibrium constant expression is written as

$$K = [CO_2] ,$$

since $CaCO_3(s)$ and $CaO(s)$ are both solids.

Problem 5. Write the equilibrium expressions for the following:

a) $C(s) + H_2O(g) \rightleftharpoons CO(g) + H_2(g)$

b) $H_2(g) + \frac{1}{2} O_2(g) \rightleftharpoons H_2O(l)$

c) $H_2(g) + S(s) \rightleftharpoons H_2S(g)$

d) $2\ C_2H_6(g) + 7\ O_2(g) \rightleftharpoons 4\ CO_2(g) + 6\ H_2O(l)$

The CM Project

The Computer-enriched Module (CM) project is a collaborative effort by 19 faculty members in the disciplines of chemistry, mathematics and physics, to produce self-instructional computer-based materials at the introductory college level in those disciplines. Each module is designed to be usable in an academic environment with minimal computational facilities, and by students, and faculty who are not programming experts. It may be used as an adjunct to standard textual materials, or in many cases, as a replacement for them. The primary aim of each module is to use the computer in such a way that students may take a more active role in the development and discovery of concepts and phenomena.

CM Project Staff

Chemistry

C. J. Jameson
Chem. Group Leader
U. of Ill. - CC
Chicago, IL

M. Bader
Moravian College
Bethlehem, PA

A. K. Jameson
Loyola University
Chicago, IL

J. Manock
Western Carolina U.
Cullowhee, NC

R. T. O'Neill
Xavier University
Cincinnati, OH

F. A. Settle, Jr.
Va. Military Inst.
Lexington, VA

R. Williams
(formerly) U. of Neb.
Lincoln, NB

Mathematics

J. H. Mayne
Math. Group Leader
Loyola University
Chicago, IL

R. A. Alo
Carnegie-Mellon U.
Pittsburgh, PA

N. C. Harbertson
Cal. St. Univ.
Fresno, CA

L. C. Leinbach
Gettysburg College
Gettysburg, PA

J. C. Mathews
Iowa State Univ.
Ames, IA

L. E. Mauland
U. of North Dakota
Grand Forks, ND

Physics

H. Weinstock
Phys. Group Leader
IIT
Chicago, IL

D. Davidson
Pima Comm. Coll.
Tucson, AR

P. Goldstein
Jersey City St. C.
Jersey City, NJ

W. Lang
MacMurray College
Jacksonville, IL

L. E. Turner, Jr.
Pacific Union Coll.
Angwin, CA

S. L. Wiley
Cal. State Univ.
Dominguez Hills, CA

Address all correspondence to

Professor H. Weinstock
Director, CM Project
Physics Department
Illinois Institute of Technology
Chicago, Illinois 60616

TEACHER'S GUIDE TO
A MODULE ON CHEMICAL EQUILIBRIUM
UNIT 1. INTRODUCTION TO CHEMICAL EQUILIBRIUM

JOHN J. MANOCK
WESTERN CAROLINA UNIVERSITY

a computer-enriched module
for introductory chemistry
featuring the programs
EQSIM
KEQ

Supported by grants from the
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Exxon Foundation

TEACHER'S GUIDE TO UNIT ON INTRODUCTION TO CHEMICAL EQUILIBRIUM OF THE CHEMICAL EQUILIBRIUM MODULE

EDUCATIONAL OBJECTIVES

The purpose of this module is to have students discover the concept of equilibrium from simulated empirical data. For this reason it is important that the students encounter this before a lecture. The module is designed around the two computer programs, EQSIM and KEQ. Using these two computer programs in an interactive environment plus working the problems in the text in a self-paced manner, the student should complete this module with (1) a qualitative understanding of chemical equilibrium, (2) an ability to write an equilibrium expression for any chemical reaction, and (3) an ability to predict the direction a reaction will proceed to achieve equilibrium.

IMPLEMENTATION

As with the other modules in this group, this module may either be used as augmentation to the lecture material or as a self-contained unit. It is estimated that the student should master the material presented in this module in two hours including approximately fifteen minutes of terminal time.

ANSWERS TO PROBLEMS

1. a) $K = \frac{[NH_2]^2}{[H_2]^3[N_2]}$

   b) $K = \frac{[SO_3][NO]}{[SO_2][NO_2]}$

   c) $K = \frac{[NO_2]^2}{[O_2][NO]^2}$

2. a) Reactants
   b) Products
   c) Products

3. a) Form products
   b) Form products

4. a) Form reactants
   b) Form reactants

5. a) $K = \frac{[CO][H_2]}{[H_2O]}$

   b) $K = \frac{1}{[H_2][O_2]^{1/2}}$

   c) $K = \frac{[H_2S]}{[H_2]}$

   d) $K = \frac{[CO_2]^4}{[O_2]^7[C_2H_6]^2}$

SOFTWARE

EQSIM. This computer program simulates a gaseous system: $A \rightleftharpoons B + C$ achieving equilibrium. The student is asked to supply three different time values. The program sorts these time values in ascending order, and presents four pictures of the system as functions of time, including time 0.00 minutes.

The positions of the gaseous molecules, A, B, and C, are randomly placed in order for the student to feel as though the system were dynamic. The first picture shows 20 A molecules. The next three pictures show 15, 5, 5; 8, 12, 12; 8, 12, 12 A, B, and C molecules, respectively. After the student has observed these pictures, the equilibrium is approached from the other side of the reaction starting with B and C molecules. Again, the same approach is followed with the student supplying the time values. However, in this case the four pictures are 0, 20, 20; 5, 15, 15; 8, 12, 12; 8, 12, 12 A, B, and C molecules, respectively. Make certain that students count the total number of molecules.

The main impetus of this computer program is for the student to gain an intuitive feeling for a dynamic equilibrium. By counting the gaseous molecules he should note the similarities and differences between the different pictures as the equilibrium is approached from both sides.

KEQ. This computer program provides simulated data which the student uses to derive an empirical expression for the equilibrium concentrations. The first example chosen is the simple system $A \rightleftharpoons B + C$ without emphasizing the fact the volume is included in the concentration terms. The student is asked to find an expression of the equilibrium concentrations which is independent of $A_{(initial)}$. Various combinations of the equilibrium concentrations are presented to him by the computer program, he selects one of these, and the computer program plots the quantity as a function of $A_{(initial)}$.

After he has discovered the equilibrium expression, a more complicated system $A \rightleftharpoons 2B$ is presented. Now, he must consider coefficients and volume dependencies. Again, he is asked to choose an expression which he feels is independent of $A_{(initial)}$. He selects one of these and the computer program plots this quantity as a function of $A_{(initial)}$. The emphasis of the module is for the student to be led into a quantitative understanding of an equilibrium expression through the exciting mode of discovery.

```
**THE CONCEPT OF EQUILIBRIUM**

   THE PURPOSE OF THIS PROGRAM IS TO AID YOU IN
UNDERSTANDING THE CONCEPT OF EQUILIBRIUM.  THE GASEOUS
REACTION DISCUSSED IS
          A <=> B + C
FOUR PICTURES WILL BE SHOWN WHICH WILL REPRESENT THE SYSTEM
AS TIME CHANGES, BEGINNING WITH TIME, T = 0.
CHOOSE THREE TIMES (IN MINUTES AFTER TIME ZERO) THAT YOU
WOULD LIKE TO SEE, AND ENTER THESE TIMES (SEPARATED BY
COMMAS) AFTER THE QUESTION MARK APPEARS -- E.G. ? 2,4,6

PLEASE ENTER THREE TIMES IN ASCENDING ORDER?10,15,20

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
◆            A    A  ◆
◆    A               ◆
◆ A        A         ◆
◆      A            A◆
◆         A          ◆
◆    A     A         ◆
◆      A     A       ◆
◆        AA AA A  A  ◆
◆                    ◆
◆       A           A◆
◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆

   TIME IS  0    MINUTES.

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
◆     BA             ◆
◆                    ◆
◆      A      C      ◆
◆               B    ◆
◆    A    A          ◆
◆ A          A       ◆
◆ AB  B     AAB A    ◆
◆                    ◆
◆C AC   A C    A A A ◆
◆                    ◆
◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆

   TIME IS  10   MINUTES.

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
◆        B    C      ◆
◆            C       ◆
◆     C   C  B     C ◆
◆            B B   B ◆
◆A    A   A          ◆
◆ B           C     A◆
◆ACB C  B    B      A◆
◆B         A      B  ◆
◆      B            C◆
◆A  B          C    C◆
◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆

   TIME IS  15   MINUTES.
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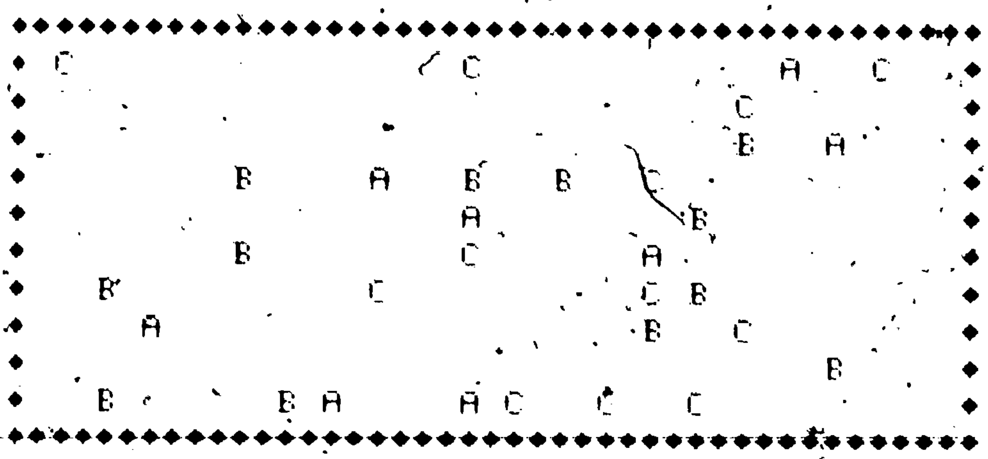
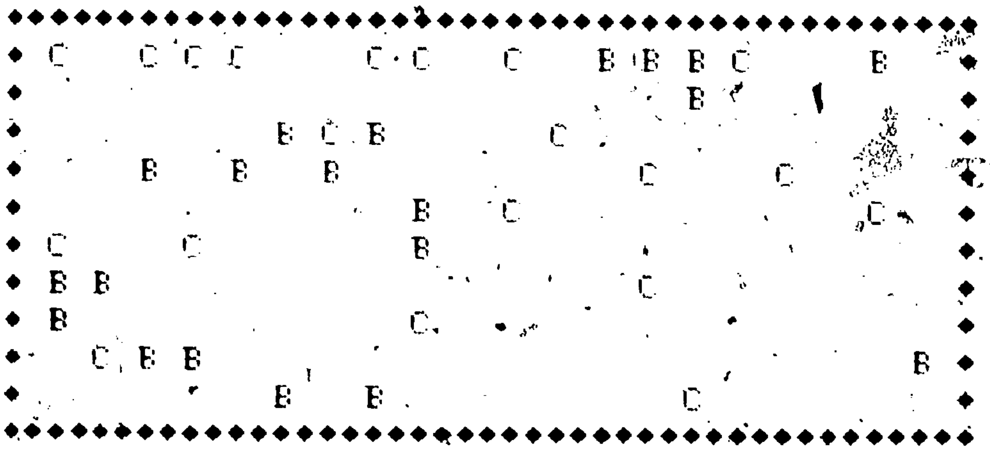


TIME IS 20 MINUTES.

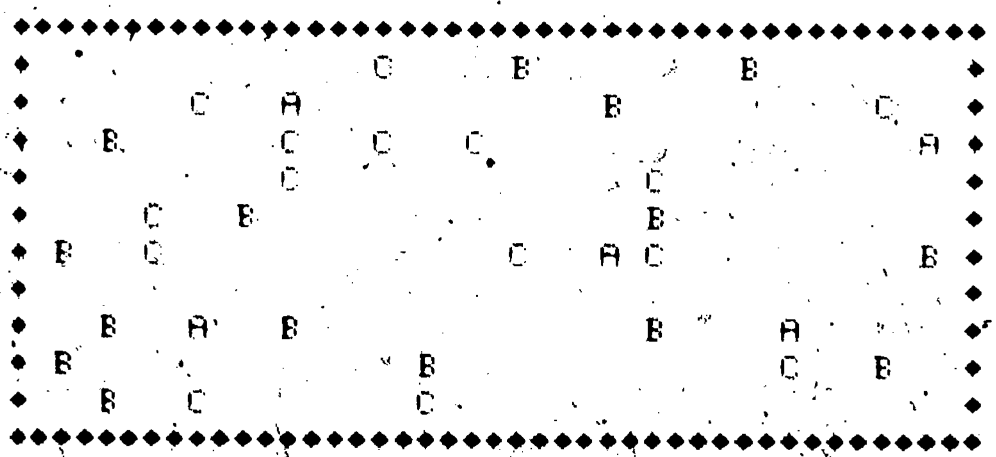
HOW DO THESE PICTURES DIFFER? HOW ARE THEY SIMILAR? ANSWER THESE QUESTIONS IN YOUR STUDENT GUIDE OR ON A SEPARATE PIECE OF PAPER.

NOW LET US CONSIDER STARTING WITH SUBSTANCES B AND C AND OBSERVE HOW THE SYSTEM ATTAINS EQUILIBRIUM. AS BEFORE, CHOOSE THREE TIMES YOU WISH TO OBSERVE.

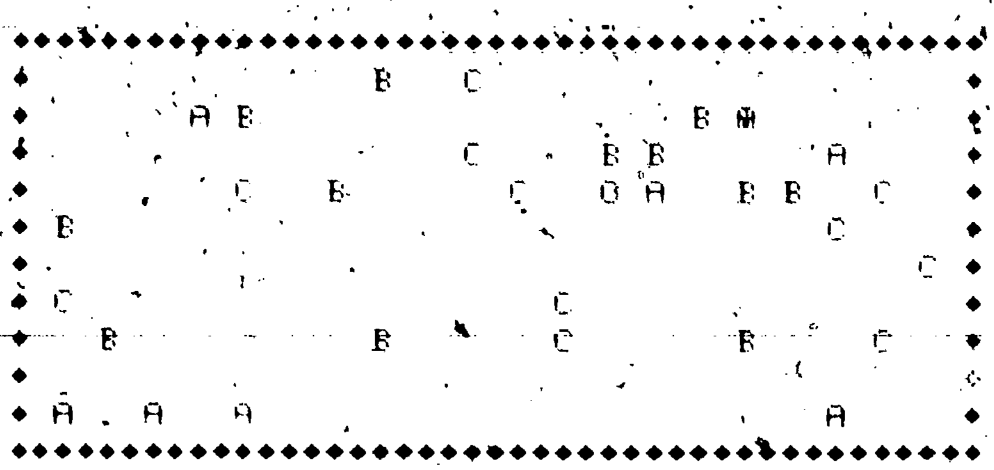
PLEASE ENTER THREE TIMES IN ASCENDING ORDER?10,15,20



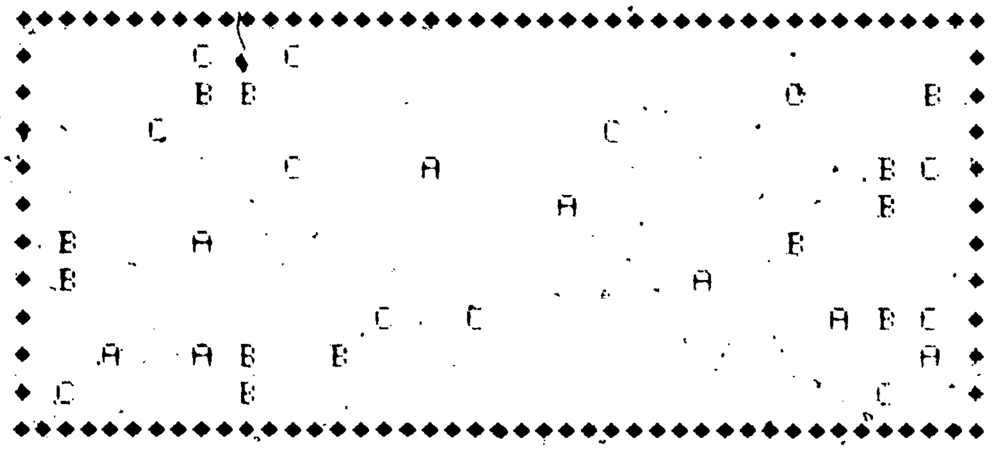
TIME IS 0 MINUTES.



TIME IS 10 MINUTES.



TIME IS 15 MINUTES.



TIME IS 20 MINUTES.

HOW DO THESE PICTURES DIFFER? HOW ARE THEY SIMILAR? ANSWER THESE QUESTIONS IN YOUR STUDENT GUIDE OR ON A SEPARATE PIECE OF PAPER.

Sample run of KEQ (BASIC version)

```
   THIS PROGRAM IS DESIGNED TO HELP THE STUDENT
EMPIRICALLY DERIVE THE EQUILIBRIUM EXPRESSION AND
GAIN INSIGHT INTO THE CONCEPT OF CHEMICAL EQUILIBRIUM.
GIVEN THE CHEMICAL EQUATION :
        A = B + C
THE FOLLOWING EXPERIMENTAL RESULTS WERE OBSERVED (WITH
CONCENTRATIONS BEING IN MOLES PER LITER.)
   A(INITIAL)   A(EQ)      B(EQ)      C(EQ)
     10          2.679      7.32       7.32
     7           1.508      5.492      5.492
     5           .858       4.142      4.142
     3           .351       2.649      2.649
     2           .168       1.832      1.832
  IT IS POSSIBLE TO FIND A RELATION AMONG THE EQUILIBRIUM
CONCENTRATIONS WHICH DOES NOT CHANGE AS A(INITIAL)
IS CHANGED. TRY VARIOUS COMBINATIONS OF THE EQUILIBRIUM
CONCENTRATIONS OF A(INITIAL) TO FIND AN EXPRESSION THAT
IS INVARIANT. FOR EXAMPLE, A(EQ) VERSUS A(INITIAL) :
   I                    O
   I
   I
   I           O
   I
   I       O
   I
   I
   I   O
   IO
   ********************
        A(INITIAL) -->
OBVIOUSLY THIS CHANGES, SHOWING THAT A(EQ) IS
DEPENDENT UPON  A(INITIAL).
  FROM THE FOLLOWING TABLE, SELECT THE EXPRESSION YOU
WOULD EXPECT TO BE INDEPENDENT OF A(INITIAL).
     (1) A*B                   (2) B^2
     (3) (C*B)/A               (4) C + B
     (5) C/A                   (6) C + B + A
     (7) OTHER
WHAT NUMBER DO YOU SELECT?1
   I                    O
   I
   I
   I
   I           O
   I
   I
   I       O
   I
   IO  O
   ********************
        A(INITIAL) -->
THIS INCREASES MORE THAN A(EQ) AS A FUNCTION OF
A(INITIAL).   TRY AGAIN.
```

```
WHAT NUMBER DO YOU SELECT?3
  IO  O  ) O    O      O
  I
  I
  I
  I
  I
  I
  I
  I
  I
 ********************
       A(INITIAL) -->
```

THIS IS CORRECT. YOU CAN PROCEED TO THE SECOND PART

YOU HAVE SHOWN THAT FOR THE REACTION:

A = B + C

THAT B(EQ)*C(EQ)/A(EQ) = A CONSTANT

REGARDLESS OF THE INITIAL CONCENTRATION OF THE REACTANT, A.

NOW CONSIDER ANOTHER GASEOUS REACTION :

A = 2B

WHERE BOTH THE INITIAL CONCENTRATION OF A AND THE VOLUME OF THE SYSTEM ARE OBSERVED.

1 VOLUME (LITERS)	2 A(INITIAL)	3 A(EQ)	4 B(EQ)	5 A(EQ)	6 B(EQ)
	*************	(MOLES)	************	**(MOLES/LITER)**	
2	3.5	2.45	2.1	1.225	1.05
2	10	8.092	3.816	4.046	1.908
3	5	3.47	3.06	1.15667	1.02
3	7	5.138	3.724	1.71267	1.24133
4	4	2.5	3	.625	.75
4	8.5	6.148	4.704	1.537	1.176

WHERE COLUMNS 2,3, AND 4 ARE EXPRESSED IN MOLES,AND COLUMNS 5 AND 6 IN MOLES PER LITER.

DETERMINE WHICH OF THE FOLLOWING EXPRESSIONS IS A CONSTANT INDEPENDENT OF A(INIT) AND VOLUME.

(1) (COLUMN 4)/(COLUMN 3)
(2) (COLUMN 4) SQUARED / (COLUMN 3)
(3) (COLUMN 6) SQUARED / (COLUMN 5)
(4) (COLUMN 6)/(COLUMN 3)
(5) OTHER

```
WHAT NUMBER DO YOU SELECT?1
  I  O
  I
  I
  I
  IO    O
  I          O
  I       O
  I
  I
  I            O
 ********************
       A(INITIAL) -->
```

THE FIRST TWO ROWS SHOW THAT THIS IS FALSE. TRY AGAIN.

```
WHAT NUMBER DO YOU SELECT?2
  I  O            O
  I
  I
  I
  I
  I     O     O
  I
  I
  I
  IO                   O
  ◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
         A(INITIAL) -->
COMPARE ANY TWO ROWS WITH APPROXIMATELY THE SAME
CONCENTRATION --E.G. ROWS 3 AND 4.  TRY AGAIN.
WHAT NUMBER DO YOU SELECT?4
  I  O
  I
  I
  I
  IO    O
  I               O
  I           O
  I
  I
  I                    O
  ◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
         A(INITIAL) -->
NO. COMPARE ROWS 3 AND 4.   TRY AGAIN.
WHAT NUMBER DO YOU SELECT?3
  IO O  O     O   O    O
  I
  I
  I
  I
  I
  I
  I
  I
  I
  ◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
         A(INITIAL) -->
THIS IS CORRECT.  CONGRATULATIONS!!!
```

Sample run of KEQ (FORTRAN version)

THIS PROGRAM IS DESIGNED TO HELP THE STUDENT EMPIRICALLY DERIVE THE EQUILIBRIUM EXPRESSION AND GAIN INSIGHT INTO THE CONCEPT OF CHEMICAL EQUILIBRIUM.
GIVEN THE FOLLOWING CHEMICAL REACTION:

A = B + C

THE FOLLOWING EXPERIMENTAL RESULTS WERE OBSERVED.(CONC. IN MOLES/LITER)

A(INITIAL)	A(EQ)	B(EQ)	C(EQ)
10.0	2.679	7.320	7.320
7.0	1.508	5.492	5.492
5.0	.858	4.142	4.142
3.0	.351	2.649	2.649
2.0	.168	1.832	1.832

IT IS POSSIBLE TO FIND A RELATION AMONG THE EQUILIBRIUM CONCS.WHICH DOES NOT CHANGE AS A(INITIAL) IS CHANGED.TRY VARIOUS COMBINATIONS OF THE EQUIL. CONCS. AS FUNCTIONS OF A(INITIAL) TO FIND AN EXPRESSION WHICH IS INVARIANT.

FOR EXAMPLE: A(EQ) VERSUS A(INITIAL)

```
I                        0
I
I
I               0
I
I         0
I
I
I   0
I0
 *********************
   A(INITIAL)
```

OBVIOUSLY, THIS CHANGES SHOWING THAT A(EQ) IS DEPENDENT UPON A(INITIAL)

FROM THE FOLLOWING TABLE SELECT THE EXPRESSION YOU WOULD EXPECT TO BE INDEPENDENT OF A(INITIAL).

```
   (1)    (A*B)        (2)    (B**2)
   (3)    (C*B)/A      (4)    (C+B)
   (5)    (C/A)        (6)    (C+B+A)
   (7)    OTHER
ENTER YOUR SELECTION.1
```

```
 I                    O
 I
 I
 I
 I            O
 I
 I
 I       O
 I
 IO O
  *********************
    A(INITIAL)
THIS INCREASES MØRE THAN A(EQ) AS A
FUNCTIØN ØF A(INITIAL)
TRY AGAIN
ENTER YØUR SELECTIØN.2

 I                    O
 I
 I
 I
 I            O
 I
 I
 I       O
 I
 IO O
  *********************
    A(INITIAL)
THIS INCREASES MØRE THAN A(EQ) AS A
FUNCTIØN ØF A(INITIAL)
TRY AGAIN
ENTER YØUR SELECTIØN.4

 I                    O
 I
 I
 I            O
 I
 I       O
 I
 I
 I  O
 IO
  *********************
    A(INITIAL)
THIS IS A CØMMØN MISTAKE BECAUSE ØF
STØICHIØMETRY.NØTE THE INCREASE.
TRY AGAIN
ENTER YØUR SELECTIØN.5
```

```
 IO
 I
 I
 I
 I  O
 I
 I
 I       O
 I            O
 I                    O
  ********************
    A(INITIAL)
THIS FUNCTIØN DECREASES
TRY AGAIN
ENTER YØUR SELECTIØN.6

 I                    O
 I
 I
 I            O
 I
 I
 I       O
 I
 I  O
 IO
  ********************
    A(INITIAL)
THIS IS A CØMMØN MISTAKE BECAUSE ØF
STØICHIØMETRY.NØTE THE INCREASE.
TRY AGAIN
ENTER YØUR SELECTIØN.3

 IO O    O    O       O
 I
 I
 I
 I
 I
 I
 I
 I
 I
  ********************
    A(INITIAL)
THIS IS CØRRECT. PRØCEED TØ 2ND PART.
YØU HAVE SHØWN THAT FØR THE REACTIØN:

      A  =  B + C

  B(EQ)C(EQ)/A(EQ) = CØNSTANT

REGARDLESS ØF THE INITIAL CØNCENTRATIØN
ØF REACTANT A
```

NØW CØNSIDER ANØTHER TYPE ØF GASEØUS RX.

A = 2B

WHERE BØTH THE INITIAL CØNCENTRATIØN ØF A AND THE VØLUME ØF THE SYSTEM ARE VARIED. THE FØLLØWING EXPERIMENTAL RESULTS WERE ØBSERVED.

1	2	3	4	5	6
VØLUME	A(INIT)	A(EQ)	B(EQ)	A(EQ)	B(EQ)
LITERS	(	MØLES	)	(MØLES/LITER)	
2.	3.50	2.450	2.100	1.225	1.050
2.	10.00	8.092	3.816	4.046	1.908
3.	5.00	3.470	3.060	1.157	1.020
3.	7.00	5.138	3.724	1.713	1.241
4.	4.00	2.500	3.000	.625	.750
4.	8.50	6.148	4.704	1.537	1.176

WHERE CØLUMNS 2,3,SAND 4 ARE EXPRESSED IN MØLES AND CØLUMNS 5 AND 6 IN MØLES/LITER. DETERMINE WHICH ØF THE FØLLØWING EXPRESSIØNS IS A CØNSTANT, INDEPENDENT ØF A(INT) AND VØL.

```
    (1)   4/3         (2)    (4**2)/3
    (3)  6**2/5       (4)     6/5
    (5)  ØTHER
ENTER YØUR SELECTIØN.4

 I 0
 I
 I
 I
 I0   0
 I              0
 I         0
 I
 I
 I                   0
  ********************
    A(INITIAL)
NØ, CØMPARE RØWS 3 AND 4
TRY AGAIN

NTER YØUR SELECTIØN.2

 I 0            0
 I
 I
 I
 I
 I    0     0
 I
 I
 I
 I0                  0
  ********************
    A(INITIAL)
```

```
COMPARE ANY TWO ROWS WITH APPROX.
THE SAME CONC.,E.G. ROWS 3 & 4
TRY AGAIN
ENTER YOUR SELECTION.3

 I00  0     0     0     0
 I
 I
 I
 I
 I
 I
 I
 I
 I
  *********************
     A(INITIAL)
THIS IS CORRECT. CONGRATULATIONS.
 END OF PROGRAM
```

EQSIM Program (in BASIC)

```
30 REM ******************** P R O G R A M ****************************
90 REM INSERT THE ARGUMENT FOR RND WHICH YIELDS A REPEATING RANDOM NO.
100 REM SEQUENCE IN STATEMENT 140.
110 REM ************************************************************
120 REM
130 REM--> FNR SHOULD GENERATE A REPRODUCIBLE SEQUENCE.
140 DEF FNR(N)=RND(N)
150 LET N=FNR(-1)
160 REM--- K0 IS THE GRAPH LENGTH,IT SHOULD BE <= S2 OF ARRAY L IN DIM
170 DIM T[4],L[10,20]
180 LET K0=20
190 DATA 20,15,8,8,0,5,8,8
200 LET S=0
210 PRINT            TAB(14);"**THE CONCEPT OF EQUILIBRIUM**";LIN(1)
220 PRINT "     THE PURPOSE OF THIS PROGRAM IS TO AID YOU IN"
230 PRINT "UNDERSTANDING THE CONCEPT OF EQUILIBRIUM.  THE GAS EOUS"
240 PRINT "REACTION DISCUSSED IS";LIN(1);TAB(15);"A <=> B + C"
250 PRINT "FOUR PICTURES WILL BE SHOWN WHICH WILL REPRESENT THE SYSTEM"
260 PRINT "AS TIME CHANGES, BEGINNING WITH TIME, T = 0."
270 PRINT "CHOOSE THREE TIMES (IN MINUTES AFTER TIME ZERO) THAT YOU"
280 PRINT "WOULD LIKE TO SEE, AND ENTER THESE TIMES (SEPARATED BY"
290 PRINT "COMMAS) AFTER THE QUESTION MARK APPEARS -- E.G. ? 2,4,6"
300 GOTO 340
310 PRINT "     NOW LET US CONSIDER STARTING WITH SUBSTANCES"
320 PRINT "B AND C AND OBSERVE HOW THE SYSTEM ATTAINS EQUILIBRIUM."
330 PRINT "AS BEFORE, CHOOSE THREE TIMES YOU WISH TO OBSERVE."
340 PRINT LIN(1);"PLEASE ENTER THREE TIMES IN ASCENDING ORDER";
350 LET T[1]=0
360 INPUT T[2],T[3],T[4]
370 IF T[2]>=T[3] OR T[3]>=T[4] THEN 340
380 PRINT
390 LET S=S+1
400 FOR I=1 TO 4
410   READ A
420   LET B=K0-A
430   LET C=B
440   LET T=A+B+C
450   MAT L=ZER
460   REM
470   REM>>> CHOOSE RANDOM X,Y COORDINATES IN A 10*K0 BOX.
480   REM
490   FOR I1=1 TO T
500     LET S1=INT(10*FNR(1)+1)
510     LET S2=INT(K0*FNR(1)+1)
520     IF L[S1,S2]=0 THEN 550
530     LET S2=S2+1-INT((S2+1)/K0)*K0+1
540     GOTO 520
550     LET L[S1,S2]=1
560     IF I1<=A THEN 600
570     LET L[S1,S2]=2
580     IF I1<=K0 THEN 600
590     LET L[S1,S2]=3
600   NEXT I1
```

```
610   REM
620   REM>>>PRINT A PICTURE OF THE SYSTEM.
630   REM
640   GOSUB 890
650   FOR I1=1 TO 10
660     PRINT "◆ ";
670     FOR I2=1 TO K0
680       IF L[I1,I2]>0 THEN 710
690       PRINT "  ";
700       GOTO 780
710       IF L[I1,I2]>1 THEN 740
720       PRINT "A ";
730       GOTO 780
740       IF L[I1,I2]>2 THEN 770
750       PRINT "B ";
760       GOTO 780
770       PRINT "C ";
780     NEXT I2
790     PRINT "◆"
800   NEXT I1
810   GOSUB 890
820   PRINT LIN(1);TAB(5);"TIME IS";T[I];" MINUTES.";LIN(1)
830 NEXT I
840 PRINT "       HOW DO THESE PICTURES DIFFER?  HOW ARE THEY SIMILAR?"
850 PRINT "ANSWER THESE QUESTIONS IN YOUR STUDENT GUIDE OR ON A"
860 PRINT "SEPARATE PIECE OF PAPER.";LIN(1)
870 IF 3<2 THEN 310
880 STOP
890 REM ◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆SUBROUTINE PRINTS BORDERS ◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
900 LET N=(K0◆2)+3
910 FOR I3=1 TO N
920   PRINT "◆";
930 NEXT I3
940 PRINT " "
950 RETURN
960 END
```

EQSIM Program (in FORTRAN)

```
      DIMENSIØN NX(100),Y(100),SØRTN(100)
      DIMENSIØN A(8),B(8),C(8),T(4)
      DATA A,B,C/20.,15.,8.,8.,0.,5.,8.,8.,0.,5.,12.,12.,20.,
     115.,12.,12.,0.,5.,12.,12.,20.,15.,12.,12./
       DATA CØCL2,CØ,CL2/2HA ,2HB ,2HC /
   50 FØRMAT(1H ,' THE PURPØSE ØF THIS PRØGRAM IS TØ AID')
   62 FØRMAT(1H ,'HØW DØ THESE PICTURES DIFFER?'/)
   64 FØRMAT(1H ,' NØW LET US CØNSIDER STARTING WITH')
   65 FØRMAT(1H ,'SUBSTANCES B AND C AND ØBSERVE HØW THE')
   66 FØRMAT(1H ,'SYSTEM ØBTAINS EQUILIBRIUM. AS BEFØRE')
   67 FØRMAT(1H ,'ENTER T1,T2,AND T3 IN MINUTES')
   51 FØRMAT(1H ,'YØU IN THE UNDERSTANDING ØF THE CØNCEPT')
   52 FØRMAT(1H ,'ØF CHEMICAL EQUILIBRIUM.  THE GASEØUS')
   53 FØRMAT(1H ,'REACTIØN DISCUSSED IS: A = B + C')
   54 FØRMAT(1H ,'FØUR PICTURES WILL BE SHØWN WHICH WILL')
   55 FØRMAT(1H ,'REPRESENT THE SYSTEM AS TIME CHANGES')
   56 FØRMAT(1H ,'BEGINNING WITH TIME EQUAL ZERØ. CHØØSE')
   57 FØRMAT(1H ,'THREE TIMES(IN MINUTES) FØR WHICH YØU')
   58 FØRMAT(1H ,'WØULD LIKE TØ SEE PICTURES ØF THE SYSTEM')
   59 FØRMAT(1H ,'AND ENTER THESE TIMES: T1,T2,T3.')
   60 FØRMAT(1H ,'(INCLUDE THE DECIMAL PØINTS)')
   61 FØRMAT(1H ,'    T1    T2    T3'/)
   63 FØRMAT(1H ,'HØW ARE THESE PICTURES SIMILIAR?'/)
      NS=4
      M1=1
      M2=4
      NV=20
      WRITE(6,50)
      NCØUNT=0
      WRITE(6,51)
      WRITE(6,52)
      WRITE(6,53)
      WRITE(6,54)
      WRITE(6,55)
      WRITE(6,56)
      WRITE(6,57)
      WRITE(6,58)
      WRITE(6,59)
      T(1)=0.
      LS=5
      WRITE(6,60)
      N1=2
      XP=123.
      WRITE(6,61)
    5 READ(5,91)(T(I),I=N1,NS)
   91 FØRMAT(3F5.0)
      DØ 3 I=1,4
```

```
      NX(I)=0
    3 Y(I)=0.
      CALL SØRT(NX,Y,T,4)
      DØ 99 KO=M1,M2
      NA=A(KO)
      NB=B(KO)
      NC=C(KO)
      NTØT=NA+NB+NC
           DØ 11 I=1,NA
   11 Y(I)=CØCL2
      NS=NA+1
      NT=NA+NB
      DØ 12 I=NS,NT
   12 Y(I)=CØ
      NS=NA+NB+1
      DØ 13 I=NS,NTØT
   13 Y(I)=CL2
      DØ 14 I=1,NTØT
      CALL JØHN (XP,YZL)
      NX(I)=NV*YZL + 1
      CALL JØHN(XP,YZL)
   14 SØRTN(I)=YZL
      CALL SØRT(NX,Y,SØRTN,NTØT)
      CALL PLØT(NX,Y,SØRTN,NV,NTØT,T(LS-KO))
   99 CØNTINUE
       WRITE(6,62)
      WRITE(6,63)
      IF(NCØUNT.EQ.1)STØP
      NS=4
      N1=2
      M2=8
      M1=5
      NCØUNT=NCØUNT+1
      LS=9
      WRITE(6,64)
      WRITE(6,65)
      WRITE(6,66)
      WRITE(6,67)
      WRITE(6,61)
      T(1)=0.0
      GØ TØ 5
      END
      SUBRØUTINE SØRT(NX,Y,SØRTN,NTØT)
      DIMENSIØN NX(1),Y(1),SØRTN(1)
      NM=NTØT-1
      DØ 1 J=1,NM
      KØ=J+1
      DØ 1 K=KØ,NTØT
      IF(SØRTN(K).LT.SØRTN(J))GØ TØ 1
      SS=SØRTN(K)
      YS=Y(K)
      NS=NX(K)
      Y(K)=Y(J)
      NX(K)=NX(J)
```

```
          SØRTN(K)=SØRTN(J)
          Y(J)=YS
          SØRTN(J)=SS
          NX(J)=NS
    1     CØNTINUE
          RETURN
          END
          SUBRØUTINE PLØT(NX,Y,SØRTN,NV,NTØT,T)
          DIMENSIØN NX(1),Y(1),BØX(25),SØRTN(1),NES(25)
          DATA BLANK,SLASH,SINE/2H  ,2H* ,2H**/
          DØ 1 I=1,25
    1     BØX(I)=BLANK
          NVP=NV+2
          DØ 2 I=1,NVP
    2     BØX(I)=SINE
          BØX(NV+3)=SLASH
          WRITE(6,5)(BØX(I),I=1,23)
    5     FØRMAT(1H ,23A2)
          DØ 3 I=1,25
    3     BØX(I)=BLANK
          K=1
          DØ 7 L=1,10
          IC=0
          BØX(1)=SLASH
          BØX(NV+3)=SLASH
          IF(K.GT.NTØT) GØ TØ 6
           TEST=1.-.1*L
    4     IF(SØRTN(K).LT.TEST)GØ TØ 6
          IF(IC.EQ.0)GØ TØ 16
   14     DØ 18 II=1,IC
   15     IF(NES(II).EQ.(NX(K)+1))GØ TØ 17
   18     CØNTINUE
   16     BØX(NX(K)+1)=Y(K)
          IC=IC+1
          NES(IC)=NX(K)+1
          K=K+1
          IF(K.GT.NTØT)GØ TØ 6
          GØ TØ 4
   17     IF(NX(K).EQ.22)NX(K)=1
          NX(K)=NX(K)+1
          GØ TØ 14
    6     WRITE(6,5)(BØX(I),I=1,23)
           DØ 8 M=1,25
    8     BØX(M)=BLANK
    7     CØNTINUE
          DØ 20 II=1,IC
   20     NES(II)=0
          DØ 10 I=1,NVP
   10     BØX(I)=SINE
          BØX(NV+3)=SLASH
          WRITE(6,5)(BØX(I),I=1,23)
          WRITE(6,11)T
   11     FØRMAT(1H ,5X,'TIME IS',F6.2,' MINUTES'/)
          RETURN
          END
```

```
      SUBRØUTINE JØHN(X,F)
      X=131.*X
       I=X/16384.
      XI=I
      X=X-XI*16384.
      F=X/16384.
      RETURN
      END
```

KEQ Program (In BASIC)

```
>LIST

 10 REM    KEQ  BY JOHN MANDOCH, WESTERN CAROLINA U.
 20 REM WRITTEN AT ILLINOIS INSTITUTE OF TECHNOLOGY(CHICAGO) .
 30 REM AS PART OF A MODULE ON CHEMICAL EQUILIBRIUM.
 40 REM TRANSLATED FROM FORTRAN TO "STANDARD" BASIC BY
 50 REM R.T.O'NEILL, XAVIER UNIVERSITY (CINCINNATI) JAN. 1975
 60 REM  FOR SYSTEMS THAT USE CRT'S (INSTEAD OF PAPER OUTPUT DEVICES)
 70 REM IT IS SUGGESTED THAT LINES 2380,2570,2660, AND 2740 READ
 80 REM  'GOTO 2200', AND THAT LINES 3560,3670,3860 READ 'GOTO 3100'
 90 PRINT "    THIS PROGRAM IS DESIGNED TO HELP THE STUDENT"
100 PRINT "EMPIRICALLY DERIVE THE EQUILIBRIUM EXPRESSION AND"
110 PRINT "GAIN INSIGHT INTO THE CONCEPT OF CHEMICAL EQUILIBRIUM."
120 PRINT "GIVEN THE CHEMICAL EQUATION :"
130 PRINT "              A = B + C"
140 PRINT "THE FOLLOWING EXPERIMENTAL RESULTS WERE OBSERVED (WITH"
150 PRINT "CONCENTRATIONS BEING IN MOLES PER LITER.)"
160 PRINT TAB(4);"A(INITIAL)";TAB(16);"A(EQ)";TAB(24);
170 PRINT "B(EQ)";TAB(32);"C(EQ)"
180 DIM B[22],C[22]
190 FOR I=1 TO 5
200   READ X[I],A[I],B[I]
210   LET P[I]=X[I]
220   LET O[I]=B[I]
230   PRINT TAB(4);X[I];TAB(16);A[I];TAB(24);B[I];TAB(32);B[I];
240   PRINT
250 NEXT I
260 DATA 10,2.679,7.32,7,1.508,5.492,5,.858,4.142
270 DATA 2,.351,2.649,2,.168,1.832
280 PRINT "   IT IS POSSIBLE TO FIND A RELATION AMONG THE EQUILIBRIUM"
290 PRINT "CONCENTRATIONS WHICH DOES NOT CHANGE AS A(INITIAL)"
300 PRINT "IS CHANGED. TRY VARIOUS COMBINATIONS OF THE EQUILIBRIUM"
310 PRINT "CONCENTRATIONS OF A(INITIAL) TO FIND AN EXPRESSION THAT"
320 PRINT "IS INVARIANT. FOR EXAMPLE, A(EQ) VERSUS A(INITIAL) :"
330 LET N=5
340 GOSUB 1730
350 PRINT "OBVIOUSLY THIS CHANGES, SHOWING THAT A(EQ) IS"
360 PRINT "DEPENDENT UPON  A(INITIAL)."
370 PRINT "  FROM THE FOLLOWING TABLE, SELECT THE EXPRESSION YOU"
380 PRINT "WOULD EXPECT TO BE INDEPENDENT OF A(INITIAL)."
390 PRINT "       (1) A*B                     (2) B^2"
400 PRINT "       (3) (C*B)/A                 (4) C + B"
410 PRINT "       (5) C/A                     (6) C + B + A"
420 PRINT "       (7) OTHER"
430 PRINT "WHAT NUMBER DO YOU SELECT";
440 INPUT S
450 GOTO S OF 460,460,540,610,690,760,830
460 FOR I=1 TO 5
470   LET P[I]=B[I]*B[I]
480 NEXT I
490 GOSUB 1600
500 GOSUB 1730
510 PRINT "THIS INCREASES MORE THAN A(EQ) AS A FUNCTION OF"
520 PRINT "A(INITIAL).    TRY AGAIN."
530 GOTO 430
```

```
540 FOR I=1 TO 5
550   LET O[I]=20
560 NEXT I
570 GOSUB 1600
580 GOSUB 1730
590 PRINT "THIS IS CORRECT.  YOU CAN PROCEED TO THE SECOND PART"
600 GOTO 860
610 FOR I=1 TO 5
620   LET O[I]=2*B[I]
630 NEXT I
640 GOSUB 1600
650 GOSUB 1730
660 PRINT "THIS IS A COMMON MISTAKE BECAUSE OF STOICHIOMETRY."
670 PRINT "NOTE THE INCREASE.    TRY AGAIN."
680 GOTO 430
690 FOR I=1 TO 5
700   LET O[I]=B[I]/A[I]
710 NEXT I
720 GOSUB 1600
730 GOSUB 1730
740 PRINT "THIS FUNCTION DECREASES.    TRY AGAIN."
750 GOTO 430
760 FOR I=1 TO 5
770   LET O[I]=A[I]+2*B[I]
780 NEXT I
790 GOSUB 1600
800 GOSUB 1730
810 PRINT &
    "THIS IS A COMMON MISTAKE BECAUSE OF STOICHIOMETRY. TRY AGAIN"
820 GOTO 430
830 PRINT "DISCUSS THIS WITH YOUR INSTRUCTOR."
840 GOTO 2130
850 END
860 PRINT
870 PRINT "  YOU HAVE SHOWN THAT FOR THE REACTION:"
880 PRINT "               A = B + C"
890 PRINT "THAT         B(EQ)*C(EQ)/A(EQ)  =  A CONSTANT"
900 PRINT "REGARDLESS OF THE INITIAL CONCENTRATION OF THE REACTANT  A."
910 PRINT
920 PRINT "   NOW CONSIDER ANOTHER GASEOUS REACTION :"
930 PRINT "                  A = 2B"
940 PRINT "WHERE BOTH THE INITIAL CONCENTRATION OF A AND THE VOLUME"
950 PRINT "OF THE SYSTEM ARE OBSERVED."
960 PRINT "1";TAB(9);"2";TAB(23);"3";TAB(33);
970 PRINT "4";TAB(47);"5";TAB(58);"6"
980 PRINT "VOLUME";TAB(9);"A(INITIAL)";TAB(23);"A(EQ)";TAB(33);
990 PRINT "B(EQ)";TAB(47);"A(EQ)";TAB(58);"B(EQ)"
1000 PRINT "(LITERS)";TAB(9);"************(MOLES)************";
1010 PRINT TAB(47);"**(MOLES/LITER)**"
1020 FOR I=1 TO 6
1030   READ R1[I],R2[I],R3[I]
1040   LET Z1=R2[I]-R3[I]
1050   LET Z2=2*R3[I]
1060   PRINT R1[I];TAB(9);R2[I];TAB(23);Z1;TAB(33);
1070   PRINT Z2;TAB(47);Z1/R1[I];TAB(58);Z2/R1[I]
1080 NEXT I
1090 LET N=6
```

```
1100 DATA 2,3.5,1.05,2,10,1.908,3,5,1.53
1110 DATA 3,7,1.862,4,4,1.5,4,8.5,2.352
1120 PRINT "WHERE COLUMNS 2,3, AND 4 ARE EXPRESSED IN MOLES,AND COLUMNS"
1130 PRINT "5 AND 6 IN MOLES PER LITER."
1140 PRINT "    DETERMINE WHICH OF THE FOLLOWING EXPRESSIONS IS A"
1150 PRINT "CONSTANT INDEPENDENT OF A(INIT) AND VOLUME."
1160 PRINT "       (1)      (COLUMN 4)/(COLUMN 3)"
1170 PRINT "       (2)      (COLUMN 4) SQUARED / (COLUMN 3)"
1180 PRINT "       (3)      (COLUMN 6) SQUARED / (COLUMN 5)"
1190 PRINT "       (4)      (COLUMN 6)/(COLUMN 3)"
1200 PRINT "       (5) OTHER"
1210 PRINT "WHAT NUMBER DO YOU SELECT";
1220 INPUT S
1230 FOR I=1 TO 6
1240   LET P[I]=R2[I]
1250 NEXT I
1260 GOTO S OF 1270,1340,1420,1490,1560
1270 FOR I=1 TO 6
1280   LET O[I]=2*R3[I]/(R2[I]-R3[I])
1290 NEXT I
1300 GOSUB 1600
1310 GOSUB 1730
1320 PRINT "THE FIRST TWO ROWS SHOW THAT THIS IS FALSE.  TRY AGAIN."
1330 GOTO 1210
1340 FOR I=1 TO 6
1350   LET O[I]=(2*R3[I])**2/(R2[I]-R3[I])
1360 NEXT I
1370 GOSUB 1600
1380 GOSUB 1730
1390 PRINT "COMPARE ANY TWO ROWS WITH APPROXIMATELY THE SAME"
1400 PRINT "CONCENTRATION --E.G. ROWS 3 AND 4.  TRY AGAIN."
1410 GOTO 1210
1420 FOR I=1 TO 6
1430   LET O[I]=(2*R3[I]/R1[I])**2/((R2[I]-R3[I])/R1[I])
1440 NEXT I
1450 GOSUB 1600
1460 GOSUB 1730
1470 PRINT "THIS IS CORRECT.  CONGRATULATIONS!!!"
1480 GOTO 2130
1490 FOR I=1 TO 6
1500   LET O[I]=(2*R3[I]/R1[I])/((R2[I]-R3[I])/R1[I])
1510 NEXT I
1520 GOSUB 1600
1530 GOSUB 1730
1540 PRINT "NO. COMPARE ROWS 3 AND 4.    TRY AGAIN."
1550 GOTO 1210
1560 PRINT "DISCUSS THIS WITH YOUR INSTRUCTOR."
1570 GOTO 2130
1580 REM
1590 REM  SUBROUTINE SORT
1600 FOR J=1 TO N-1
1610   K0=J+1
```

```
1620   FOR K=K0 TO N
1630     IF Q[J]>Q[K] THEN 1700
1640     LET Q9=Q[J]
1650     LET P9=P[J]
1660     LET Q[J]=Q[K]
1670     LET P[J]=P[K]
1680     LET Q[K]=Q9
1690     LET P[K]=P9
1700   NEXT K
1710 NEXT J
1720 RETURN
1730 REM
1740 REM SUBROUTINE PLOT
1750 LET Q5=(Q[1]-Q[N])/10
1760 IF Q5<.0001 THEN Q5=1
1770 LET Q9=Q[1]
1780 LET P9=P[1]
1790 LET P0=P[1]
1800 FOR J=1 TO N
1810   IF P[J]>P9 THEN P9=P[J]
1820   IF P[J]<P0 THEN P0=P[J]
1830 NEXT J
1840 LET P5=(P9-P0)/20
1850 LET L=1
1860 FOR J=1 TO 10
1870   LET B$="I"
1880   FOR K=1 TO 21
1890     LET C[K]=0
1900   NEXT K
1910   LET T5=Q9-J*Q5
1920   IF L>N THEN 1980
1930   IF Q[L]<T5 THEN 1980
1940   LET N5=(P[L]-P0)/P5+.1
1950   LET C[N5+1]=1
1960   LET L=L+1
1970   GOTO 1920
1980   FOR K=1 TO 21
1990     IF C[K]=1 THEN 2020
2000     LET B$=B$+" "
2010     GOTO 2030
2020     LET B$=B$+"O"
2030   NEXT K
2040   PRINT TAB(2);B$
2050 NEXT J
2060 PRINT TAB(2);
2070 FOR J=1 TO 20
2080   PRINT "*";
2090 NEXT J
2100 PRINT
2110 PRINT "          A(INITIAL) -->"
2120 RETURN
2130 END
>
```

32-B

KEQ Program (in FORTRAN)

```
      DIMENSIØN X(5),Y(6),A(5),B(5),R1(6),R2(6),R3(6)
      DIMENSIØN Z(6)
      DATA X,A,B/10.,7.,5.,3.,2.,2.679,1.508,.858,.351,
     /.168,7.320,5.492,4.142,2.649,1.832/
      DATA R1,R2,R3/2.,2.,3.,3.,4.,4.,3.5,10.,5.0,7.,4.,
     /8.5,1.05,1.908,1.530,1.862,1.5,2.352/
  100 FØRMAT(1H ,' THIS PRØGRAM IS DESIGNED TØ HELP THE')
  101 FØRMAT(1H ,'STUDENT EMPIRICALLY DERIVE THE ')
  102 FØRMAT(1H ,'EQUILIBRIUM EXPRESSIØN AND GAIN INSIGHT')
  103 FØRMAT(1H ,'INTØ THE CØNCEPT ØF CHEMICAL EQUILIBRIUM.')
  104 FØRMAT(1H ,'GIVEN THE FØLLØWING CHEMICAL REACTIØN:')
  105 FØRMAT(1H ,'          A  =  B  +  C')
  106 FØRMAT(1H ,'THE FØLLØWING EXPERIMENTAL RESULTS WERE')
  107 FØRMAT(1H ,'ØBSERVED.(CØNC. IN MØLES/LITER)')
  108 FØRMAT(1HO,'   A(INITIAL)  A(EQ)   B(EQ)   C(EQ)')
  109 FØRMAT(1HO,' IT IS PØSSIBLE TØ FIND A RELATIØN AMØNG')
  110 FØRMAT(1H ,' THE EQUILIBRIUM CØNCS.WHICH DØES NØT')
  111 FØRMAT(1H ,'CHANGE AS A(INITIAL) IS CHANGED.TRY')
  112 FØRMAT(1H ,'VARIØUS CØMBINATIØNS ØF THE EQUIL. CØNCS.')
  113 FØRMAT(1H ,'AS FUNCTIØNS ØF A(INITIAL) TØ FIND AN')
  114 FØRMAT(1H ,'EXPRESSIØN WHICH IS INVARIANT.')
  115 FØRMAT(1HO,'FØR EXAMPLE: A(EQ) VERSUS A(INITIAL)'/)
  116 FØRMAT(1HO,'ØBVIØUSLY, THIS  CHANGES SHØWING THAT')
  117 FØRMAT(1H ,'A(EQ) IS DEPENDENT UPØN A(INITIAL)')
  118 FØRMAT(1HO,'FRØM THE FØLLØWING TABLE SELECT THE')
  119 FØRMAT(1H ,'EXPRESSIØN YØU WØULD EXPECT TØ BE')
  120 FØRMAT(1H ,'INDEPENDENT ØF A(INITIAL).')
  121 FØRMAT(1HO,'    (1)    (A*B)       (2)   (B**2)')
  122 FØRMAT(1H ,'    (3)   (C*B)/A      (4)   (C+B)')
  123 FØRMAT(1H ,'    (5)   (C/A)        (6)   (C+B+A)')
  124 FØRMAT(1H ,'    (7)   ØTHER')
  125 FØRMAT(1H ,'ENTER YØUR SELECTIØN.')
  126 FØRMAT(1H ,'THIS INCREASES MØRE THAN A(EQ) AS A')
  127 FØRMAT(1H ,'FUNCTIØN ØF A(INITIAL)')
  128 FØRMAT(1H ,'THIS IS CØRRECT. PRØCEED TØ 2ND PART.')
  129 FØRMAT(1H ,'THIS IS A CØMMØN MISTAKE BECAUSE ØF')
  130 FØRMAT(1H ,'TRY AGAIN')
  131 FØRMAT(1H ,'STØICHIØMETRY.NØTE THE INCREASE.')
  132 FØRMAT(1H ,'THIS FUNCTIØN DECREASES')
  201 FØRMAT(1H ,'YØU HAVE SHØWN THAT FØR THE REACTIØN:')
  202 FØRMAT(1HO,'          A  =  B + C')
  203 FØRMAT(1HO,'  B(EQ)C(EQ)/A(EQ) = CØNSTANT')
  204 FØRMAT(1HO,'REGARDLESS ØF THE INITIAL CØNCENTRATIØN')
  205 FØRMAT(1H ,'ØF REACTANT A')
  206 FØRMAT(1HO,' NØW CONSIDER ANØTHER TYPE ØF GASEØUS RX.')
  207 FØRMAT(1HO,'          A  =   2B')
  208 FØRMAT(1HO,'WHERE BØTH THE INITIAL CØNCENTRATIØN ØF A')
  209 FØRMAT(1H ,'AND THE VØLUME ØF THE SYSTEM ARE VARIED.')
  210 FØRMAT(1H ,'THE FØLLØWING EXPERIMENTAL RESULTS WERE')
  211 FØRMAT(1H ,'ØBSERVED.')
  212 FØRMAT(1HO,'   1        2        3       4        5        6')
  213 FØRMAT(1H ,'VØLUME   A(INIT)  A(EQ)  B(EQ)  A(EQ) B(EQ)')
  214 FØRMAT(1H ,' LITERS     (      MØLES     )     (MØLES/LITER)')
  215 FØRMAT(1HO,'WHERE CØLUMNS 2,3,SAND 4 ARE EXPRESSED IN')
  216 FØRMAT(1H ,'MØLES AND CØLUMNS 5 AND 6 IN MØLES/LITER.')
```

```
217   FØRMAT(1H ,'DETERMINE WHICH ØF THE FØLLØWING EXPRESSIØNS
218   FØRMAT(1H ,'IS A CØNSTANT, INDEPENDENT ØF A(INT) AND VØ
220   FØRMAT(1H ,'     (1)   4/3       (2)    (4**2)/3')
221   FØRMAT(1H ,'     (3)  6**2/5     (4)    6/5')
222   FØRMAT(1H ,'     (5)  ØTHER')
      WRITE(6,100)
      WRITE(6,101)
      WRITE(6,102)
      WRITE(6,103)
      WRITE(6,104)
      WRITE(6,105)
      WRITE(6,106)
      WRITE(6,107)
      WRITE(6,108)
      DØ 1 I=1,5
  1   WRITE(6,134)X(I),A(I),B(I),B(I)
134   FØRMAT(1H ,F6.1,4X,F10.3,2F8.3)
      WRITE(6,109)
      WRITE(6,110)
       WRITE(6,111)
      WRITE(6,112)
      WRITE(6,113)
      WRITE(6,114)
      WRITE(6,115)
      CALL PLØT(X,B,5)
      WRITE(6,116)
      WRITE(6,117)
      WRITE(6,118)
      WRITE(6,119)
      WRITE(6,120)
      WRITE(6,121)
      WRITE(6,122)
      WRITE(6,123)
      WRITE(6,124)
      WRITE(6,125)
  2   READ(5,135)INDEX
135   FØRMAT(I1)
      IF(INDEX-4)10,11,12
 10   IF(INDEX-2)7,7,9
 12   IF(INDEX-6)13,14,15
  7   DØ 17 I=1,5
      Z(I)=X(I)
 17   Y(I)=B(I)*B(I)
      CALL SØRT(Z,Y,5)
      CALL PLØT(Z,Y,5)
      WRITE(6,126)
      WRITE(6,127)
      WRITE(6,130)
      WRITE(6,125)
      GØ TØ 2
  9   DØ 19 I=1,5
      Z(I)=X(I)
 19   Y(I)=20.
      CALL SØRT(Z,Y,5)
```

```
      CALL PLØT(Z,Y,5)
      WRITE(6,128)
      GØ TØ 199
   11 DØ 21 I=1,5
      Z(I)=X(I)
   21 Y(I)=2*B(I)
      CALL SØRT(Z,Y,5)
      CALL PLØT(Z,Y,5)
      WRITE(6,129)
      WRITE(6,131)
      WRITE(6,130)
      WRITE(6,125)
      GØ TØ 2
   13 DØ 23 I=1,5
      Z(I)=X(I)
   23 Y(I)=B(I)/A(I)
      CALL SØRT(Z,Y,5)
      CALL PLØT(Z,Y,5)
      WRITE(6,132)
      WRITE(6,130)
      WRITE(6,125)
      GØ TØ 2
   14 DØ 24 I=1,5
      Z(I)=X(I)
   24 Y(I)=A(I)+2*B(I)
      CALL SØRT(Z,Y,5)
      CALL PLØT(Z,Y,5)
      WRITE(6,129)
      WRITE(6,131)
      WRITE(6,130)
      WRITE(6,125)
      GØ TØ 2
   15 WRITE(6,136)
  136 FØRMAT(1H ,'DISCUSS THIS WITH YØUR INSTRUCTØR.')
      GØ TØ 280
  199 CØNTINUE
      WRITE(6,201)
      WRITE(6,202)
      WRITE(6,203)
      WRITE(6,204)
      WRITE(6,205)
      WRITE(6,206)
      WRITE(6,207)
      WRITE(6,208)
      WRITE(6,209)
      WRITE(6,210)
      WRITE(6,211)
      WRITE(6,212)
      WRITE(6,213)
      WRITE(6,214)
      DØ 300 I=1,6
      Z1=R2(I)-R3(I)
```

```
123.97            Z2=2*R3(I)
123.98            Z3=Z1/R1(I)
123.99            Z4=Z2/R1(I)
123.991   300     WRITE(6,225)R1(I),R2(I),Z1,Z2,Z3,Z4
123.992   225     FØRMAT(1H ,F4.0,6X,F6.2,2X,4F6.3)
123.993           WRITE(6,215)
123.994           WRITE(6,216)
123.995           WRITE(6,217)
123.996           WRITE(6,218)
123.997           WRITE(6,220)
123.998           WRITE(6,221)
123.999           WRITE(6,222)
124.1             WRITE(6,125)
124.2     250     READ(5,251)INDEX
124.3     251     FØRMAT(I1)
124.4             IF(INDEX-2)260,261,262
124.5     262     IF(INDEX-4)263,264,265
124.6     260     DØ 270 I=1,6
124.8             Y(I)=2.*R3(I)/(R2(I)-R3(I))
124.81    270     Z(I)=R2(I)
124.9             CALL SØRT(Z,Y,6)
124.91            CALL PLØT(Z,Y,6)
124.92            WRITE(6,226)
124.921   226     FØRMAT(1H ,'FIRST TWØ RØWS SHØWS THIS IS FALSE')
124.922           WRITE(6,130)
124.923           WRITE(6,125)
124.924           GØ TØ 250
124.93    261     DØ 271 I=1,6
124.94            Y(I)=(2.*R3(I))**2/(R2(I)-R3(I))
124.95    271     Z(I)=R2(I)
124.96            CALL SØRT(Z,Y,6)
124.97            CALL PLØT(Z,Y,6)
124.98            WRITE(6,227)
124.981           WRITE(6,228)
124.982   227     FØRMAT(1H ,'CØMPARE ANY TWØ RØWS WITH APPRØX.')
124.983   228     FØRMAT(1H ,'THE SAME CØNC.,E.G. RØWS 3 & 4')
124.984           WRITE(6,130)
124.985           WRITE(6,125)
124.986           GØ TØ 250
124.99    263     DØ 273 I=1,6
124.991           Y(I)=(2.*R3(I)/R1(I))**2/((R2(I)-R3(I))/R1(I))
124.992   273     Z(I)=R2(I)
124.993           CALL SØRT(Z,Y,6)
124.994           CALL PLØT(Z,Y,6)
124.995           GØ TØ 279
124.996   264     DØ 274 I=1,6
124.997           Y(I)=(2.*R3(I)/R1(I))/((R2(I)-R3(I))/R1(I))
124.998   274     Z(I)=R2(I)
124.999           CALL SØRT(Z,Y,6)
125               CALL PLØT(Z,Y,6)
125.1             WRITE(6,231)
125.11    231     FØRMAT(1H ,'NØ. CØMPARE RØWS 3 AND 4')
125.12            WRITE(6,130)
125.13            WRITE(6,125)
125.14            GØ TØ 250
125.2     265     WRITE(6,136)
```

```
279     WRITE(6,229)
229     FØRMAT(1H ,'THIS IS CØRRECT. CØNGRATULATIØNS.')
280     STØP
        END
        SUBRØUTINE SØRT(X,Y,NPTS)
        DIMENSIØN X(1),Y(1)
        NM=NPTS-1
        DØ 5 J=1,NM
        KØ=J+1
        DØ 5 K=KØ,NPTS
        IF(Y(J).GE.Y(K))GØ TØ 5
        YS=Y(J)
        XS=X(J)
        Y(J)=Y(K)
        X(J)=X(K)
        Y(K)=YS
        X(K)=XS
  5     CØNTINUE
        RETURN
         END
        SUBRØUTINE PLØT(X,Y,NPTS)
        DIMENSIØN X(1),Y(1),BØX(25)
        DATA BLANK,SLASH,STAR,CIRCLE/1H ,1HI,1H*,1HO/
        YSCAL=(Y(1)-Y(NPTS))/10.
        IF(YSCAL.LT..0001)YSCAL=1.
        YMAX=Y(1)
        XMAX=X(1)
        XMIN=X(1)
        DØ 2 J=1,NPTS
        IF(X(J).GT.XMAX)XMAX=X(J)
  2     IF(X(J).LT.XMIN)XMIN=X(J)
        XSCAL=(XMAX-XMIN)/20.
        L=1
        DØ 10 J=1,10
        DØ 6 K=2,22
  6     BØX(K)=BLANK
        BØX(1)=SLASH
        SL=J
        TEST=YMAX-SL*YSCAL
  7     IF(L.GT.NPTS)GØ TØ 10
        IF(Y(L).LT.TEST)GØ TØ 10
        N=(X(L)-XMIN)/XSCAL+.1
        BØX(N+2)=CIRCLE
        L=L+1
        GØ TØ 7
 10     WRITE(6,15)(BØX(I),I=1,22)
 15     FØRMAT(1H ,1X,22A1)
        DØ 11 J=1,20
 11     BØX(J)=STAR
        WRITE(6,16)(BØX(I),I=1,20)
 16     FØRMAT(1H ,2X,20A1)
        WRITE(6,17)
 17      FØRMAT(1H ,'    A(INITIAL)')
        RETURN
        END
```