

AD-780 301

PHAS20, A PROGRAM FOR SIMULTANEOUS MULTIPLE
REGRESSION OF A MATHEMATICAL MODEL TO THERMO-
CHEMICAL DATA

GEOLOGICAL SURVEY

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GEOLOGICAL SURVEY
COMPUTER CONTRIBUTION

USGS - GD - 74 - 018

PHAS20, A Program for Simultaneous Multiple Regression
of a Mathematical Model to Thermochemical Data

by

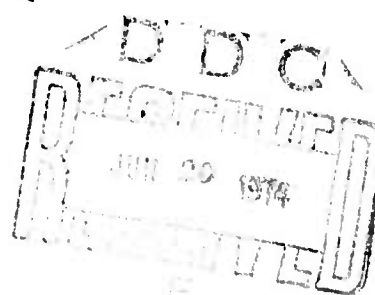
John L. Haas, Jr.

U.S. Geological Survey

Washington, D. C.

1974

Program Number: G466
Equipment: IBM 360/65
Operating System: IBM System 360
Language: FORTRAN IV



CONTENTS

Abstract	1
Introduction	1
Description	2
Data input and editing	2
Multiple regression	3
The mathematical model	3
Output of error plots and associated tabular data	4
Tables of preliminary thermodynamic values	4
Input requirements and data description	8
Run data	9
Problem data	9
Introductory data	9
Observations	11
Trial parameters	14
Plot control data	16
Choosing trial parameters	16
Constraints	17
Constraints derived from a reference state	17
Constraints derived from a phase transition	18
Use of the subroutine PRELIM	19
Use of the subroutine UNIQUE	19
Program run preparation	20
Output	21
The printed output	21
Listing of input data sets	21
Regression results	21
Printer plots	22
Preliminary tables of thermochemical data and the refined parameters	22
The punched output	22
Explanation of error messages	23
Glossary of main FORTRAN	24
Acknowledgements	29
References	30

Attachment A. Example of the use of the subroutine UNIQUE . . .	31
Attachment B. Examples of an execution of PHAS20 . . .	36
Problem 1. The System H_2O and the self-ionization of water . . .	37
Listing of input deck	37
Printed output	42
Problem 2. The System Ni-O and the thermodynamics of Bunsenite (NiO)	79
Listing of input deck	79
Printed output	82
Attachment C. Listing of PHAS20 and associated routines . . .	118
PHAS20	119
BLOCK DATA	129
ORGLS2	130
PRELIM	136
TEST20	137
MINV20	139
EAFW20	141
YDERIV	145
DDERIV	149
DIE	150
FN	151
UNIQUE	152
PUTOUT	153
PRPLOT	155

ABSTRACT

PHAS20 performs simultaneous multiple regression of a mathematical model for the functional relations among thermodynamic quantities to experimental data for a group of chemically related species. The thermodynamic quantities included are heat capacity, entropy, enthalpy, free energy, equilibrium constant, electrochemical potential, and relative heat content. Without further adjustment, PHAS20 will fit the model to 70 sets of data containing a total of 1200 observations on 20 species. The data may include any and all of the following types of observations:

For individual species:

1. heat capacity
2. third law entropy
3. enthalpy of formation from oxides and elements
4. free energy of formation from oxides and elements
5. relative heat content data such as are obtained from by drop calorimetry

For reactions:

1. heat capacity change
2. entropy change
3. enthalpy change
4. enthalpy change of a transition (e.g., heat of fusion, heat of vaporization, etc.)
5. free energy change
6. equilibrium constant
7. electrochemical potential

INTRODUCTION

The ideal compilation of thermochemical data, as yet unrealized, would be both complete and accurate. The approach to completion is a function only of the assiduity of the experimentalist and is therefore beyond the reach of data compilers. Assessment of the accuracy of a thermochemical datum, however, requires knowledge of the precision of its experimental determination as well as its consistency with other equivalent measurements and with thermochemical data functionally related to it. This program automatically fits to the data a mathematical model consistent with the exact functional relations among heat capacity (C_p), entropy (S), enthalpy (H), free energy (G), equilibrium constant (K), and electrochemical potential (E) for a group of chemically related species. The program then returns a "best set" of species-related constants from which further thermodynamic calculations may be made or compilations assembled. These are accomplished by the following steps:

1. All or selected data, weighted by the reciprocal of their precision, are fitted to a mathematical model which is consistent with the thermodynamic theory for a group of chemically related species.
2. Error plots for each data set (grouped by type and reference source) are supplied.

3. The user examines the error plots and removes the discordant data sets.
4. The program is rerun and a new fit of the mathematical model to the revised data is obtained.
5. Error plots for each data set are again supplied as a check upon the decisions made in step 3.
6. Preliminary table of thermodynamic values for each species in the chemical system is printed. As a second test, these values can be compared against existing compilation to insure all thermodynamic parameters have reasonable values.
7. At the option of the user, step-backward elimination of non-significant parameters in the mathematical model will cause repeating of steps 4, 5, and 6 for each parameter deleted. The maximum number of steps to be taken is set by the user. However, if the variance in all the parameters drops below 10 percent, elimination will also stop.

DESCRIPTION

The program PHAS20 is divided into 4 major parts; 1) data input and editing, 2) multiple regression, 3) output of error plots and associated tubular data, and 4) output of tables of preliminary thermodynamic values.

Data input and editing

The units of observations found in the literature are varied. Successful analysis requires a standard set of units. In PHAS20 the accepted units are as follows:

<u>Parameters or Thermodynamic Property</u>	<u>Units</u>
temperature	kelvin
pressure	set by user through the data selection
heat capacity	joules mole ⁻¹ kelvin ⁻¹
entropy	joules mole ⁻¹ kelvin ⁻¹
enthalpy	joules mole ⁻¹
free energy	joules mole ⁻¹
equilibrium constant	logarithm (base 10)
electrochemical potential	volt

Provision is made in PHAS20 to accept most data in the units given by the reference source. The temperature is edited by the following equation:

$$T(K) = T(\text{input}) + T(\text{factor}) \quad (1)$$

where $T(\text{factor})$ is defined by the user. In most instances $T(\text{factor})$ will have a value 273.15 where temperatures are converted from the centigrade scale to the kelvin scale. Pressure is not an input variable. To change the units for thermodynamic properties equation 2 is used:

$$Y(\text{units given in above listing}) = Y(\text{input}) \times Y(\text{factor}) \quad (2)$$

where Y is any thermodynamic observation and Y(factor) is the conversion factor from the published units to the units used in PHAS20. This procedure simplifies input preparation because most data can be punched directly from the source and edited on input by PHAS20.

Multiple regression

Multiple regression of the mathematical model described below to the data is accomplished by the subroutines ORGLS2 and MINV20. These have been adopted from the Oak Ridge general least squares regression program by Busing and Levy (1962). The changes in the above program were those necessary to adapt it to the peculiar problem encountered here. Since all changes are superficial, the reader is referred to the report by Busing and Levy for the description of the routines.

The Mathematical Model

Thermodynamic theory provides the following exact functional relations among the heat capacity (C_p), entropy (S), enthalpy (H), free energy (G), equilibrium constant (K), and electrochemical potential (E):

$$S_i = \int \frac{C_{p_i}}{T} dT \quad (3)$$

$$H_i = \int C_{p_i} dT \quad (4)$$

$$G_i = H_i - T S_i \quad (5)$$

$$-R T \ln K = \sum_{i=1}^k s_i G_i \quad (6)$$

$$-n F E = \sum_{i=1}^k s_i G_i \quad (7)$$

where T is the thermodynamic temperature, R and F are the ideal gas constant and the faraday, respectively, k is the number of species in the reaction and s is the stoichiometric coefficient, positive for products and negative for reactants. From these it follows that an empirical relation which adequately defines C_{p_i} as a function of T will generate the mathematical description of the other thermodynamic parameters. For non-aqueous species, equation (8) has been adopted:

$$C_{p_i} = a_i + 2 b_i T + \frac{c_i}{T^2} + f_i T^2 + g_i / \sqrt{T} \quad (8)$$

This is an extension of the Maier-Kelley equation (Maier and Kelley, 1932), the last two terms being added to describe adequately very

accurate data.

For aqueous ions equation (9) has been adopted:

$$C_{p,i,aq} = a_i + 2b_i T + \frac{c_i}{T^2} + f_i T^2 + -g_i \frac{T}{\epsilon} \left[\alpha^2 \exp^2 (\beta + \alpha T) + \alpha^2 \exp(\beta + \alpha T) + \frac{2\alpha}{\theta} \exp(\beta + \alpha T) + \frac{1}{\theta^2} \right] \quad (9)$$

where ϵ is the dielectric constant for liquid H_2O and is given by equation (10):

$$\epsilon = \epsilon_0 \exp \left[-\exp (\beta + \alpha T) - \frac{T}{\theta} \right] \quad (10)$$

The terms ϵ_0 , β , α , and θ are fitted constants. Equations (9) and (10) are adopted from Helgeson (1967) but retain the original terms in the Maier-Kelley equation (the first three terms in the product of equation (9)).

Table 1 gives the mathematical model as a function of temperature describing commonly available thermodynamic observations. For further discussion the reader is referred to Fisher and Haas (1973) and subsequent reports presently in preparation.

Output of error plots and associated tabular data

After the successful multiple regression of the mathematical model to fit the data, the refined parameters are used to calculate the following statistical data for all observations in each data set:

- 1) difference, $Y(obs) - Y(calc)$
 - 2) percent error, $100 \times (Y(obs) - Y(calc)) / Y(obs)$
 - 3) weighted difference, $(Y(obs) - Y(calc)) / \text{standard derivation of the experimental observation}$
 - 4) arithmetic mean for each of the above type of errors
 - 5) standard error of each of 1 thru 3 about the respective means
- 4 for the data set.

As a guide to the quality of agreement, the weighted difference is best. The weighted difference is the number of standard errors the calculated value departs from the experimentally determined value. The weighted difference is graphed against temperature on the error plots.

The PRPLOT routine used in PHAS20 was written by Carnahan and Evans (1961).

Tables of preliminary thermodynamic values

The last portion of PHAS20 calculates and prints tables for each species in the group of the chemical system. The tables contain the following (the definition are given by the equations):

TABLE 1. THE MATHEMATICAL MODEL

A. Formulae for one nonaqueous species:

$$Cp_i = a_i + 2 b_i T + \frac{c_i}{T^2} + f_i T^2 + \frac{g_i}{\sqrt{T}} \quad (A1)$$

$$S_i = a_i \ln T + 2 b_i T - \frac{c_i}{2T^2} + e_i + f_i \frac{T^2}{2} - \frac{2 g_i}{\sqrt{T}} \quad (A2)$$

$$H_i = a_i T + b_i T^2 - \frac{c_i}{T} + d_i + f_i \frac{T^3}{3} + 2 g_i \sqrt{T} \quad (A3)$$

$$G_i = a_i (T - T \ln T) - b_i T^2 - \frac{c_i}{2T} + d_i - e_i T - f_i \frac{T^3}{6} + 4 g_i \sqrt{T} \quad (A4)$$

B. Formulae for one aqueous species:

$$Cp_{i,aq} = a_i + 2 b_i T + \frac{c_i}{T^2} + f_i T^2 - g_i \frac{1}{\epsilon} \left[\alpha^2 \exp^2(\beta + \alpha T) + \alpha^2 \exp(\beta + \alpha T) + \frac{2\alpha}{\theta} \exp(\beta + \alpha T) + \frac{1}{\theta^2} \right] \quad (B1)$$

$$S_{i,aq} = a_i \ln T + 2 b_i T - \frac{c_i}{2T^2} + e_i + f_i \frac{T^2}{2} - g_i \frac{1}{\epsilon} \left[\alpha \exp(\beta + \alpha T) + \frac{1}{\theta} \right] \quad (B2)$$

$$H_{i,aq} = a_i T + b_i T^2 - \frac{c_i}{T} + d_i + \frac{f_i T^3}{3} + g_i \frac{1}{\epsilon} \left[1 - T \alpha \exp(\beta + \alpha T) - \frac{T}{\theta} \right] \quad (B3)$$

$$G_{i,aq} = a_i (T - T \ln T) - b_i T^2 - \frac{c_i}{2T} + d_i - e_i T - f_i \frac{T^3}{6} + \frac{g_i}{\epsilon} \quad (B4)$$

TABLE 1. Continued

$$\epsilon = \epsilon_0 \exp[-\exp(\beta + \alpha T) \frac{T}{\theta}] \quad (B5)$$

$$(\epsilon_0 = 305.7; \alpha = 0.01875; \beta = -12.741; \theta = 219)$$

C. Formula for relative heat content, H_R , where the i th and j th phase may be the same or different and the difference between T_2 and T_1 is the temperature interval over which the change in enthalpy is observed:

$$H_R = H_i(T_2) - H_j(T_1) \quad (C1)$$

D. Formula for a reaction involving k species where s_i is the stoichiometric coefficient for the i th species and is positive for products and negative for reactants:

$$\Delta C_p = \sum_{i=1}^k s_i C_{p,i} \quad (D1)$$

$$\Delta S = \sum_{i=1}^k s_i S_i \quad (D2)$$

$$\Delta H = \sum_{i=1}^k s_i H_i \quad (D3)$$

$$\Delta G = \sum_{i=1}^k s_i G_i \quad (D4)$$

$$\log K = \frac{-1}{RT \ln(10)} \sum_{i=1}^k s_i G_i \quad (D5)$$

$$E = \frac{-1}{nF} \sum_{i=1}^k s_i G_i \quad (D6)$$

E. Constraints:

For elements in the stable structural state at 298.15 K and the pre-determined reference pressure

$$G_e \equiv 0 \equiv a_e \cdot (298.15 - 298.15 \cdot \ln 298.15) - b_e \cdot (298.15)^2 - \frac{c_e}{2 \cdot 298.15} + d_e - e_e \cdot 298.15 - \frac{f_e (298.15)^3}{6} + 4 g_e \sqrt{298.15} \quad (E1)$$

TABLE 1. Continued

For two species undergoing an isochemical phase transition at T_{tr} :

$$\begin{aligned}
 G_2 - G_1 \equiv & (a_2 - a_1) (T_{tr} - T_{tr} \ln T_{tr}) \\
 & - (b_2 - b_1) T_{tr}^2 \\
 & - \frac{c_2 - c_1}{2 T_{tr}} \\
 & + (d_2 - d_1) \\
 & - (e_2 - e_1) T_{tr} \\
 & - \frac{(f_2 - f_1) T_{tr}^3}{6} \\
 & + 4 (g_2 - g_1) \sqrt{T_{tr}}
 \end{aligned}$$

heat capacity,	$C_p(T)$
entropy,	$S(T) = S_0 + \int_0^T \frac{C_p}{T} dT$
enthalpy,	$H(T) = G(T) + T S(T)$
free energy,	$G(T) = \Delta G_{f,298}^\circ + \int_{298}^T C_p dT - T \int_{298}^T \frac{C_p}{T} dT$
equilibrium constant,	$\log K = \frac{-G(T)}{2.303RT}$
electrochemical potential,	$E = \frac{-G(T)}{nF}$
relative heat content,	$H_R = \int_{298}^T C_p dT$

For nonaqueous species the data are calculated in the temperature range 273.15 to 2000K; for aqueous species the range is 273.15 to 523.15K. The last portion of each table contains the final constants from which the table was calculated.

Heat capacity, entropy, and relative heat content are equivalent to those given in standard compilations. The enthalpy of formation and free energy of formation of the species can be calculated provided the tables for the stable elemental species from which the species are compounded are also available;

$$\Delta G_f^\circ (\text{species}, T) = G (\text{species}, T) - \sum_{i=1}^k s_i G_i (\text{elemental species}, T) \quad (11)$$

$$\Delta H_f^\circ (\text{species}, T) = H (\text{species}, T) - \sum_{i=1}^k s_i H_i (\text{elemental species}, T) \quad (12)$$

where k is the number of elements in the species and s_i is the number of atoms of the i th element

INPUT REQUIREMENTS AND DATA DESCRIPTION

The data deck must contain the following information. Each item will be discussed in turn below.

Run data

Problem data

Introductory data

Observations

The Data sets

Trial Parameters

Plot control data

Run Data

The introductory data in the data deck consists of two cards containing the information tabulated below. The first column gives the number of cards needed to contain the data. The second column gives the variables on the cards. The third column gives the format for each card. And the last column gives a brief description of the variables.

<u>No. of Cards</u>	<u>Variable</u>	<u>Format</u>	<u>Description</u>
1	DATE	A8	Date or other alphanumeric identification of the run.
1	NREG	I5	Number of separate problems in the data deck.

Problem Data

The data for each problem is logically broken down into four groups: 1) introductory data, 2) observations, 3) trial parameters, and 4) plot control data.

Introductory Data. The introductory data contains from 5 to 7 cards:

<u>No. of cards</u>	<u>Variable</u>	<u>Format</u>	<u>Description</u>
1	TITLE (20)	20A4	Alphanumeric description of the problem, 80 characters
1	IDO	5I5	Options: 1 for both regression and error plots, 2 for regression only, 3 for error plots only.
	NC		Maximum number of cycles or refinements permitted on trial parameters. Usually set to 2 or 3.

<u>No. of Cards</u>	<u>Variable</u>	<u>Format</u>	<u>Description</u>
	IW		Weight control options: 0 for standard errors supplied by users, 1 for uniform standard error of 1 percent to be assigned by the program (The recip- rocal of the error is used as the weight on each datum).
	IL		Print control options: 0 for calculated results at plot time only, 1 for tabular data for each cycle of NC cycles.
	IFMOUT		Format control for punching of refined parameters. Options: 0 gives parameters in 6D12.5 format, 1 gives parameters in 7A8 format. Note: With IFMOUT=1, there is no round off between subse- quent reruns of the same or related problems.
1	LISTP	3I5	Number of chemical species in the problem; limit is 20
	ICY		Maximum number of nonsignifi- cant constants to be dropped by step-backward elimination.
	NHOLD		Numbers of parameters to be forced during step-backward elimination even though TEST20 may indicate they are non-significant. Limit is 40 parameters.
1-3	PNAME (LISTP)	10A8	8-character alphanumeric identification of each of the species in the chemical system.
1	ION (LISTP)	20I2	Type of species: 1 indicates a reference ele- mental species, 0 indicates non reference and nonaqueous species, -1 indicates aqueous species or water (H ₂ O liquid).

Observations. PHAS20, as described herein, will intercorrelate the type of data described by the equations in sections A, B, C, and D of Table 1. Suggestions for fitting the mathematical model to other types of data are described under Use of the Subroutine UNIQUE below.

The data may be grouped into a maximum of 70 data sets containing an aggregate of 1200 observations. These limits are set by the dimension statements and are readily changed. The grouping of data must be by identical type such as all the equilibrium constants for the same chemical reaction may be placed in one data set. But for convenience in sorting out discordant data it is recommended that such data sets be separated as to the source reference. Thus the equilibrium constants for the same reaction but from different sources should be separated into separate data sets and labeled completely on the data set identification card described below.

The Data Sets. The cards in the observation deck are as follows (Repeat beginning after the first card for each data set):

<u>No. of Cards</u>	<u>Variables & Dimension Control</u>	<u>Format</u>	<u>Description</u>
1	NSETS	I5	Number of separate data sets in the problem. <u>Maximum set at 70.</u>
1	REF (10, NSETS)	10A8	80-character alphanumeric description of the data in the data set.
1	NPHASE (NSETS)	6I5	Number of species described by this set. <u>Maximum set at 6.</u> For the heat capacity of a single phase, set to 1; for the reaction among 4 species, set to 4, etc.
	IKOUNT (NSETS)		Number of observations in the data set.
	IGO (NSETS)		Data type options (see Attachment B for examples): 1 for Cp and ΔC_p , 2 for S and ΔS , 3 for H and ΔH , 4 for G and ΔG , 5 for log k, 6 for E, 7 for $H_{T_2} - H_{T_1}$, 8 thru 14 optional for situations described under <u>Uses of the Subroutine UNIQUE.</u>

<u>No. of Cards</u>	<u>Variable & Dimension Control</u>	<u>Format</u>	<u>Description</u>
	ITFACT		Flag for editing of input temperatures: 0 for editing, 1 for no editing. See TFACT below.
	IPARA		Flag for editing of the dependent variable YO(I) and SIGYO(I): 0 for editing, 1 for no editing. See PARA below.
	ISIG		Flag for indicating the type of precision supplied for the observation: 0 for precision expressed as a ratio of the observed (e.g. $0.01 \times YO$), 1 for precision expressed as an absolute range (e.g., $0.02 \text{ J mol}^{-1}\text{K}^{-1}$).

For each of the NPHASE phases or species in the data set, prepare the following cards:

<u>No. of Cards</u>	<u>Variable & Dimension Control</u>	<u>Format</u>	<u>Description</u>
1	ANAME	(A8,2X, D10.3, 10X, 2I5)	8-character alphanumeric identifier of each species referred to in the data set. ANAME must be found in the species list PNAME, character for character and space for space
	COEF(NPHASE,NSETS)		Stoichiometric coefficient: 1) for species in reaction, positive for products, negative for reactants; or 2) number of moles upon which observation was made (generally 1 mole).
	ISTATE(NPHASE,NSETS)		Flag. If the species is a reference species with ΔG_f° at $298.15\text{K} \pm 0$ joules per moles, set to 1. If ion or $\text{H}_2\text{O}(l)$, set to -1, otherwise set to 0.

<u>No. of Cards</u>	<u>Variable & Dimension Control</u>	<u>Format</u>	<u>Description</u>
	NINVER(NPHASE, NSETS)		Number of inversions (equals the number of <u>lower</u> temperature modifi- cations being considered for the component). <u>Maximum is 4.</u>

If the number of inversions is zero continue with the next phase in turn or go to the next section beginning after INVPH below.
If inversions are considered, insert after the phase identification card the next two cards:

<u>No. of Cards</u>	<u>Variable & Dimension Control</u>	<u>Format</u>	<u>Description</u>
1	TINV(NPHASE, NSETS, KINVER)	(4D12.5)	Inversion temperature at which $\Delta G(\text{inversion})$ is set at 0 joules
1	INSTAT (NPHASE, NSETS)	(I5,I3, 5A8)	If a stable phase at 298.15 K is a reference species, set to 1, otherwise set to 0.
	INVSC(NPHASE NSETS)		On rare occasions there may be a stoichiometry change at a phase transformation. INVSC then contains the index of the net stoichiometry change which is found in the vector STCOEF(10) in BLOCK DATA. The reaction is: STCOEF (INVSC) PHASE1 =PHASE2.
	INVPH(NPHASE, NSETS, (KINVER + 1))		Beginning with the phase stable at 298.15K, list the succession of phases up temperature to and including the phase ANAME. (All names must be the same as found in PNAME)

After the phases and associated inversion data have been identified, give the data for the set:

<u>No. of Cards</u>	<u>Variable & Dimension Control</u>	<u>Format</u>	<u>Description</u>
IKOUNT	X(1,NO)	(6D12.5)	First independent variable, the temperature of observation.
	TFACT		Conversion factor to convert X(1,NO) (centigrade scale) to X(1,NO) (kelvin scale) by addition
	YO(NO)		Dependent variable
	PARA		Conversion factor to convert YO(NO) (any units) to YO(NO) in $J\ mol^{-1}K^{-1}$, $J\ mol^{-1}$, $\log K$ (base 10), or volts by multiplication
	SIGYO(NO)		Estimate of precision of the observation YO
	X(2,NO)		Second independent variable. For relative heat content, X(2, NO) is the reference temperature. The default is 298.15K. See <u>Uses of the Subroutine UNIQUE</u> for further discussion.

Repeat, beginning with REF (10,NSETS) until all data sets are entered. This then concludes the Observation portion of the input deck.

Trial Parameters. The third portions of the data deck contains the trial parameters:

<u>No. of Cards</u>	<u>Variable and Dimension Control</u>	<u>Format</u>	<u>Description</u>
1	IFMIN (LISTP)	(80I1)	Species-related flag to indicate the format used for each of LISTP species: 0 indicates (6D12 5/D12.5) 1 indicates (7A8) Because there is a format flag for each species, the format for the 7 trial parameters of one species may differ from that of the

<u>No. of Cards</u>	<u>Variable and Dimension Control</u>	<u>Format</u>	<u>Description</u>
1 or 2 cards per set, 1 set for each species in PNAME	P(LISTP*7)	(See IFMIN above)	next. The advantage of the second format is the elimination of roundoff between runs. Trial parameters of species sequenced as in PNAME. There are 7 parameters for each species, there must be contained on 2 cards if IFMIN=0, or 1 card if IFMIN=1. For more in- formation on parameters, See Parameter Section below.
1 or 2	KI(LISTP*7)	(80I1)	Flag to indicate whether the parameter of the same index is to be varied during re- gression of kept con- stant: 0-to be kept constant; 1-to be varied.

If NHOLD is not zero, the next card must be included; if NHOLD is zero, the trial parameter deck is completed.

<u>No. of Cards</u>	<u>Variable and Dimension Control</u>	<u>Format</u>	<u>Description</u>
1	IHOLD(NHOLD)	(40I2)	Index of parameters in P(LISTP*7) which are to be forced to remain in regression without re- gard as to the statisti- cal significance indi- cated by TEST20.

Plot Control Data. The plot control cards are as follows:

<u>No. of Cards</u>	<u>Variable and Dimension Control</u>	<u>Format</u>	<u>Description</u>
1	NHL	(4I5)	Number of horizontal lines in the plot less 1, generally set to 4.
	NSBH		Number of spaces between horizontal lines plus 1, generally set to 10.
	NVL		Number of vertical lines in the plot less 1. If the temperature range is 250K to 2000K, set to 7. This gives 250 degress per division.
	NSBV		Number of spaces between vertical lines plus 1. Generally set to 10.
1	XMAX	(3E10.3)	REAL*4 variable giving the upper bound on the x-coordinate.
	XMIN		REAL*4 variable giving the lower bound on the x-coordinate.
	YMAX		REAL*4 giving the upper bound on the y-coordinate. (YMIN=YMAX for a symmetrical graph). Generally set YMAX to 10.OEO. This allows weighted differences of ± 10 standard errors to be plotted, but retains enough resolution near ± 1 standard error to be useful.

This concludes the deck for the plot control cards and for the problem. If more than one problem is contained in the run, the TITLE card for the next problem follows the last card above.

Choosing Trial Parameters

Equations 8 and 9 contain 5 parameters to describe the heat capacity of the i th species. In almost all situations these are more than adequate, and in most problems, using all 5 parameters will cause a singularity in the matrix inversion. For these reasons it is often best to graph the heat capacity data (or relative heat content data) to determine the parameters in the heat capacity equation (or the relative heat content equation, Section C, Table 1) which probably are adequate to describe the data. If no heat capacity or relative heat content data are available, then, at most, only "a", "d", and "e" may have

non-zero values. Some overfitting can be removed by step-backward elimination.

Because successive refinements of the parameters is a feature of ORGLS 2, order-of-magnitude estimation of trial parameters is usually sufficient. The following are acceptable first estimates for the seven parameters.

Parameter	Type of Species	
	Non-aqueous	Aqueous
a	10	10^3
b	10^{-3}	10
c	10^5	10^7
d	10^4 ^{1/}	10^5
e	10	10^4
f	10^{-7}	10^{-2}
g	10^2	10^5

Constraints

There are two preprogrammed constraints. The first deals with reference species and associated reference state, and the second with phase transformations.

Constraint derived from a reference state

The most important constraint is that the free energy of the elemental species stable at the reference temperature and reference pressure is zero. (Refer to Fisher and Haas, 1973

for a discussion of the reference state convention adopted here.) For PHAS20 TREF, the reference temperature, is set at 298.15 in BLOCK DATA. The reference pressure is never explicitly defined in PHAS20 except for aqueous species. Therefore, for non-aqueous species, the user defines the reference pressure by data selection. For aqueous species the algorithm to calculate the dielectric constant for water is applicable to vapor-saturated water only. Indirectly then, the reference pressure is a sliding reference set for ions at the coexistence curve of water.

Equation (E1) of Table 1 gives the algebraic implications of a zero free energy at a TREF of 298.15 K. Equation (13) is derived from (E1).

^{1/} For reference species or species related to others by phase transformation, "d" is set to zero and not varied during the regression. See Constraints below.

$$\begin{aligned}
d_e = & a_e (298.15 \cdot \ln (298.15) - 298.15) \\
& + b_e \cdot (298.15)^2 + \frac{c_e}{2 \cdot 298.15} \\
& + e_e \cdot 298.15 + f_e \frac{(298.15)^3}{6} \\
& - 4 g_e (298.15)^{1/2}
\end{aligned} \tag{13}$$

In the subroutine EAFW20, for those phases specified as references (i.e. ISTATE or INSTAT = 1), d_e is calculated from TREF and the current value of the other parameters for the reference species. Therefore, in selecting trial parameters, SET D_e EQUAL TO 0.0 AND SET KI CORRESPONDING TO D_e TO 0.

Constraint derived from a phase transformation

At the temperature T_{tr} of a phase transformation the difference in the free energy between the coexisting phases is zero. This is stated algebraically by equation (E2) of Table 1. Equation (E2) can be rewritten so that d_2 , the "d"-constant of the high temperature phase may be calculated from the remaining 13 constants:

$$\begin{aligned}
d_2 = & (a_2 - a_1) \cdot (T_{tr} \cdot \ln(T_{tr}) - T_{tr}) + (b_2 - b_1) \cdot T_{tr}^2 \\
& + \frac{(c_2 - c_1)}{2 T_{tr}} + d_1 \\
& + (e_2 - e_1) \cdot T_{tr} + (f_2 - f_1) \cdot \frac{T_{tr}^3}{6} \\
& - 4 (g_2 - g_1) \cdot T_{tr}^{1/2}
\end{aligned} \tag{14}$$

In the subroutine EAFW20, for those phases specified as having lower temperature modifications (i.e. NINVER $\neq$ 0), d_2 is calculated from the inversion temperature T_{tr} and the current value of the other six parameters for the high temperature phase and the seven parameters for the lower temperature phase. If more than one transformation is considered, then d_1 is calculated as was d_2 using the data for successively lower temperature phases. DIMENSION statements limit the number of allowed transformations to 4.

In selecting trial parameters, SET "D" OF ALL HIGHER TEMPERATURE POLYMORPHS EQUAL TO 0.0 AND THE CORRESPONDING KI TO 0.

Use of the Subroutine PRELIM

PRELIM is a feature retained from the program of Busing and Levy (1962). In those situations 1) where the editing feature at read-in is not sufficient to convert units or prepare the data properly for regression or 2) where a temporary adjustment in weights is desired, PRELIM can be used. PRELIM is called from the subroutine ORGLS2 just prior to the beginning of the regression procedure. Therefore PRELIM presents a last chance to make an adjustment in the data used by ORGLS2 or any subsequent routine.

As supplied, PRELIM is a dummy subroutine and returns control to ORGLS2 without any change in the data.

Use of the Subroutine UNIQUE

PHAS20 is designed to allow simultaneous regression of the mathematical model given on Table 1 to a body of experimental observations for each and all species of a chemical system. In some situations, these are observations which do not fall into any of the types given on Table 1. A regression result, to be valid, must also permit accurate calculations of the latter data. The Subroutine UNIQUE is designed to allow the user to fit the model to these data also.

By way of explanation, let us consider the following problem. In the System Sulfur at pressures less than one bar, the sum of the partial pressures of the gaseous species equals the total pressure over the condensed phase, provided the vapor obeys the ideal gas law:

$$p(\text{total}) = \sum_{j=1}^8 p_j \quad (15)$$

where j indicates the number of sulphur atoms in the eight polymers existing in the sulphur gas.^{2/}

^{2/} The species S_9 , S_{10} , and S_{12} are neglected as very minor.

Equilibrium between the condensed phase and the j th gaseous species may be written

$$j S (\text{condensed}) = S_j (\text{ideal gas}) \quad (16)$$

and the equilibrium constant is

$$K_j \equiv p_j \quad (17)$$

because the activity of the condensed phase at vapor saturation is unity. Substitution of (17) into (15) gives

$$p(\text{total}) = \sum_{j=1}^8 K_j \quad (18)$$

Vapor pressure-temperature data will, therefore, provide additional constraints on the parameters a_j thru g_j which are implicit in (18).

For each datum the multiple regression routine ORGLS2 requires 1) a calculated value of the dependent variable obtained from the appropriate thermodynamic model function (i.e., the function given on Table 1), the independent variables, and the current values of the adjustable parameters a_j thru g_j and 2) the derivatives of the dependent variable with respect to each of the parameters being refined in the regression.

In cases like sulphur gas equilibria where the programmed code (given algebraically on Table 1) does not apply, the user should take the following actions:

1) Prepare the data as described under Observations above except IGO is given a value of 8 (Also 9 thru 14 are available for other constraints not included on Table 1. IGO is passed to UNIQUE in common statements and the programmer can branch in UNIQUE to the proper code to supply the requirement of 2 below).

2) The dummy routine UNIQUE is replaced by a user-coded routine UNIQUE which supplies the following:

$$a) \quad YC = \text{function}(X, P) \quad (19)$$

$$b) \quad DC_i = \frac{dYC}{dP_i} = \text{function}(X, P) \quad (20)$$

where YC, X, P, and DC are, respectively, the calculated dependent variable, the independent variables, the parameters, and the derivatives of the calculated dependent variable with respect to each of the parameters. The subscript i above varies from 1 thru NP, the number of parameters in the vector P. Use of UNIQUE for vapor pressure data in the System Sulphur is given in Attachment A.

For the mathematical model given on Table 1, the data cited by 2a and 2b are already programmed in EAFW20 and the associated routines YDERIV, DDERIV, DIE, and FN.

PROGRAM RUN PREPARATION

The following deck set-up includes OS/360 control cards as well as the problem deck requirements. The program is stored on LOADLIB; the card reader/tape (SYSIN file), the line printer/tape (SYSOUT file) and the line punch (SYSOUT = B) are the required input/output devices. The OS/360 control cards are identified by //'s in columns 1-2. Each control card must be punched on an IBM 029 keypunch or equivalent card codes must be used. The symbol "." denotes a blank card column.

- 1 User's JOB card
- 2 //step EXEC PGM=G466, REGION=250K, TIME=4
- 3 //STEPLIB DD DSN=SYS1.LOADLIB, DISP=SHR

```

4 //FTO6FOO1,DD,SYSOUT=A
5 //FTO7FOO1,DD,SYSOUT=B
6 //FTO5FOO1,DD,*
7 data deck in the following order:
  run data (2 cards)
  First Problem title (1 card)
    option codes (1 card)
    number of species, etc. (1 card)
    species names (1 to 3 cards)
    species types (1 card)
    number of data sets (1 card)
    data sets (minimum 4 cards per set; 1 reference card, 1
      option card, 1 to 6 phase cards each followed by 2
      transition data cards if applicable, and a minimum of 1
      observation card. The maximum number of sets is 70)
    option card for trial parameter-input format (1 card)
    trial parameters (1 or 2 cards per phase depending on
      option code.)
    flags for parameters to be varied (1 or 2 cards)
    indices of parameters forced during elimination (0 or 1
      card)
    plot controls (2 cards)
  Second Problem title (1 card)
    option codes (1 card)
    .
    .
    .
    .
    plot controls (2 cards) for last problem.
8 /*
9 //

```

OUTPUT

The printed output

The printed output from PHAS20 can logically be divided into four parts, each of which will be discussed below.

1) Listing of input data sets.

2) Regression results.

3) Printer plots

4) Tables of preliminary thermodynamic data and refined parameters.

For example of the printed output, refer to Attachment B.

Listing of input data sets. The first portion of the printed output contains an interpreted listing of the input data sets. The data for each set has been edited and should be in units consistent with the gas constant R and the faraday F. If this is not found to be true then the results of the regression will be of no value. The input data sets are printed by the main program PHAS20.

Regression results. The second part of the output, the results of regression begin with a listing of the regression options and the trial

parameters and ends with a listing of the correlation matrix. The regression results are printed from statements in ORGLS2 except that each reference (or data set identification) is printed from statements in EAFW20. If $IL = 1$, the results of all intermediate results will be printed. If $IL = 0$, only the references, the agreement factors, and the parameters will be printed for each refinement. The tables are self explanatory.

Printer Plots. After successful regression of the model to the data, the program forms and prints plots of the weighted difference $(YO(I)-YC)/SIGYO(I)$ as a function of the first independent variable $X(1,I)$. For convenience, tabular listings of the data and the difference $(YO(I)-YC)$, the percent error $(100.0 * (YO(I)-YC)/YO(I))$ and the weighted difference are printed just before each error plot. The mean of the errors and the standard error about the mean are also given. The error plots plus these simple statistics are useful in sorting out discordant data sets.

The tabular data are printed from commands in the main program, PHAS20. The reference for each data set is printed by EAFW20. The printer plots are generated and printed by the entry PLOT4 of PRPLOT.

Preliminary tables of thermochemical data and the refined parameters. The last part of each problem contains tabular listings of $C_{p,i}$, S_i , H_i , G_i , $\log K_i$, E_i and H_R as calculated from equations A1, A2, A3, A4, D5, D6, and C1 respectively. The terms $\log K_i$ and E_i are respectively the equilibrium constant for the formation of the i th phase at T from the elements at TREF (298.15K) and the electrochemical potential of the i th phase at T relative to the elements at TREF.

The preliminary tables are generated and printed from statements in PHAS20.

The punched output

The punched output is designed for use of the refined parameters in subsequent problems and in other programs where thermodynamic data are needed. The punched deck contains the following:

- 1 TITLE card for problem.
- 2 Number of species in problem.
- 3 Species name card(s). The 8-character alphanumeric name of each species in the problem.
- 4 The refined parameters P(LISTP*7) punched seven at a time using the format indicated by IFMOUT.
- 5 The complete refined parameters AA(LISTP*7) punched seven at a time using the format indicated by IFMOUT.
- 6 Repeat items 4 and 5 for each constant removed thru step-backward elimination.
- 7 Repeat items 1 thru 6 for each problem in the computer run.

In the refined parameters P(LISTP*7), the fourth parameter for each species will be zero if the species is a reference species ($ISTATE = 1$) or a high temperature polymorph ($NINVER \neq 0$). To use such a set of parameters, the fourth or "d" constant must be calculated according to equations (13) and (14), respectively. This set of

parameters can be used as input into further refinements or into new regressions.

In the complete refined parameters AA(LISTP*7), the fourth parameter is zero only thru elimination. In this set, as opposed to the set above, the fourth or "d" parameter has been calculated from equations 13 and 14 where applicable. This set of parameters can be used to calculate the thermodynamic values on Table 1, sections A thru D without consideration of the reference state constraint or of the parameters of other polymorphs.

EXPLANATION OF ERROR MESSAGES

If on input, the name (8-character alphanumeric label) of a species is misspelled and cannot be found in the list of names PNAME, the computer prints "I, YOUR FRIENDLY COMPUTER, DO NOW QUIT. IN YOUR nth DATA SET YOU HAVE MISTYPED THE PHASE NAME". A comparison of the names in the nth data set with the species name cards should locate the problem. Execution of the run is terminated.

"MATRIX HAS A ZERO DIAGONAL ELEMENT CORRESPONDING TO PARAMETER n OF THOSE VARIED." is generated when a diagonal element of the regression matrix is zero. Find the nth element by counting the 1's in the list of KI (NP) at the beginning of the regression results until n is reached. Because the programmed derivatives in EAFW20 will not normally be zero, is wrong information stored in KI (NP)? Is a stoichiometric coefficient zero by error? Is the user-supplied UNIQUE returning a derivative DC(n) of zero? The job is terminated by this error.

"SINGULARITY RETURNED BY THE MATRIX INVERTER" indicates the matrix is singular. Most often this is caused by gross overfitting. Check whether you are likely to need all parameters. Most often, if "c_i" and "f_i" are allowed to vary simultaneously for the ith species, a singular matrix is generated. The parameter "f_i" should be used only when there is definite curvature in the heat capacity plot at the high temperature extreme. An example is found on approaching the Curie pernt or lamda pernt with rising temperature. With this error message the problem is terminated and the next problem is run.

"SUBROUTINE TEST INDICATES THAT JOB IS TO BE TERMINATED FOR REASON 1." indicates that the change in subsequent refinements of the parameters P(I) is less than 10^{-8} . Continued refinement is generally not sound statistically. The control is returned from ORGLS2 to PHAS20 for continuation of the problem.

"***WARNING*** THE TERM SIG/(NO-NV) IS NEGATIVE. THE ABSOLUTE VALUE IS TAKEN AND THE REGRESSION CONTINUES." is self explanatory. Before you accept the results of the regression, make sure they make sense. The term SIG/(NO-NV) is used in calculating the statistics on the parameters P(NP).

"IN EAFW20 I IS GREATER THAN NO. THE NUMBER OF OBSERVATIONS. THEREFORE, I (THE COMPUTER) AM QUITTING. THE PROBLEM IS YOURS." normally cannot be generated unless NO is redefined by a user-supplied subroutine. Check common blocks in user-supplied PRELIM or UNIQUE for

NO. Make sure it was not redefined thru oversight.

"YOUR n -TH DATA SET CALLED UNIQUE FROM EAFW20, IGO(n) HAS A VALUE OF m BUT UNIQUE IS CURRENTLY UNPROGRAMMED." is most likely generated when IGO(n) has a number greater than 7 entered thru error at input. Check you data set option card. If you have programmed UNIQUE, then you may still have the dummy version in your source deck or object deck.

GLOSSARY OF MAIN FORTRAN SYMBOLS

NAME (MINIMUM DIMENSION), Definition or description

A(NPHASE, 7), In PUTOUT, local matrix containing the parameters for the data set being plotted.

A, Elsewhere, variable name assigned to the constant in the equation for the dielectric constant for water.

AA(NP), Vector containing the complete set of constants for all species in the problem.

ACOE(NPHASE, NSETS), REAL*4 variable used for output of the coefficients of a species.

AN, The number of items in a data set.

ANAME, The name (or identification) of a species, the constants of which are constrained by the associated data set. ANAME must appear in PNAME (LISTP), character for character, blank for blank and is used to find the index of the species in PNAME. The index is then used in all subsequent calculations and is assigned to the matrix IPHASE (NPHASE, LISTP).

ASTAR, Decoration for output.

AVAL(7), REAL*4 variable used to print preliminary table of thermodynamic values.

B, Variable name assigned to the constant β in the equation for the dielectric constant for water.

BCD, LOGICAL*1 variable containing the alphanumeric character used on the printer plot.

COEF(NPHASE, NSETS), Matrix of stoichiometric coefficients for reacting species in the LISTP data sets. The coefficients are negative for reactants and positive for products by convention.

CPRIME, When the constants for the reaction are printed at plot time, the constant g is separated into $g(\text{non aqueous})$ and $g(\text{aqueous})$. CPRIME contains the $g(\text{aqueous})$ summation while A((NPHASE+1),7) contains the $g(\text{non aqueous})$ summation.

D, In PUTOUT D contains the result $d_i = a_i(T \ln T - T) + b_i T^2 + c_i/2T + e_i T + f_i T^3/6 - 4g_i T^{1/2}$ where $T=298.15$, the reference temperature. The above relation is derived from the constraint (E-1) of Table 1.

DATE, 8-character alphanumeric label to identify the run. The date is suggested.

DC(NP), Vector containing the derivatives of YC with respect to the parameter P(NP).

DDDC(7), Component derivative of YC with respect to the parameters P(NP) generated by the constraints given on Table 1, section E.

DDERIV, Subroutine used to calculate DDDC.

NAME (MINIMUM DIMENSION), Definition or description

DERRP, Local variable used in TEST20.

DIE, Functions which returns the value for the dielectric constant of water at temperature T and vapor saturation.

DIEO, ϵ_0 of the equation for the dielectric constant of water.

DYDC(7), Component of derivative of YC with respect to the parameters P(NP) at the temperature of the observation (or reference temperature for relative heat content data).

E(1), The weighted difference (YO-YC)/SIGYO passed to the printer plot routine PRPLOT.

EAFW20, Subroutine which calculates YC and DC(NP).

EBAR(3), Mean of the difference, the percent error, and the weighted difference calculated at plot time for each data set.

ERR, The difference YO-YC, REAL*4 for use in output.

ERRDP, The difference YO-YC used for calculations.

ERRP(NP), The error in P(NP) calculated in ORGLS2 and used in significance test in TEST20.

F, The faraday (96487.0 C mol⁻¹).

FN, Function returning the result $FN = \exp(\beta + \alpha T)$ from the equation for the dielectric constant of water.

FNT, Result of calling FN(T).

FOUR, The value 4.0D0.

I, Local index.

ICY, Number of steps in step-backward elimination. Default = 0.

IDO, Flag to indicate operations to be executed. Options: 1 for regression and plots, 2 for regression only, 3 for plots only.

IFMIN, Flag to indicate input format for parameters P. Options: 0 for (6D12.5/D12.5), 1 for (7A8).

IFMOUT, Flag to indicate output format for parameters P. Options same as IFMIN.

IGO, Flag to indicate type of data in data set. For the types Cp, S, H, G, log K, E, and $H_{T2} - H_{T1}$, use 1 thru 7, respectively. For types programmed by the user in UNIQUE, use the unassigned flags 8 thru 14.

IGOE, Local variable having the value IGO+7 and used exclusively in call to YDERIV from EAFW20 or PHAS20.

IHOLD(NHOLD), Index of the parameters in P which are to remain in the regression during step-backward elimination without regard to significance.

II, Local index.

IICY, Flag to indicate the number of parameters dropped thru step-backward elimination.

IINVR, Local index.

IKOUNT(NSETS), At input, the number of observations in a data set. During run, IKOUNT contains the index of the last item in each data set.

IL, Flag to reduce print. Options: IL=0 for calculated results after cycle 3 or plot time only, IL=1 for calculated results after each refinement cycle.

NAME (MINIMUM DIMENSION), Definition or description

IMAGE(5000), LOGICAL*1 vector containing the plot image in vector form.

IN, Local index.

INDEX, Local index.

INDEX2, Local index.

INSTAT(NPHASE, NSETS), Flag to indicate whether the species stable at 298.15K is a reference species (=1) or not (=0).

INVPH(NPHASE, NSETS, NINVER), Index of the species in PNAME (LISTP) which are involved in polymorphic transitions.

INVSC (NPHASE, NSETS), If the polymorphic phase transformation at the highest temperature involves a stoichiometry change, find the appropriate reactant coefficient in the vector STCOEF and assign the index to INVSC:

<u>Index</u>	<u>STCOEF</u>
1	1.0D0
2	2.0D0
3	3.0D0
4	4.0D0
5	5.0D0
6	1/2.0D0
7	1/2.5D0
8	1/3.0D0
9	1/4.0D0
10	1/5.0D0

For example, consider the reaction: $2 \text{FeCl}_3(\text{liquid}) = \text{Fe}_2\text{Cl}_6$ (ideal gas). Here the reactant coefficient is 2.0 and the index 2 should be assigned to INVSC.

ID, Local index.

ION (LISTP), Flag to indicate the type of species: +1 for reference species, -1 for aqueous species and $\text{H}_2\text{O}(\text{liq})$, 0 for all other.

IPARA, Flag to indicate whether input YO and SIGYO are to be edited
IPARA=0 executes $\text{YO}=\text{YO}*\text{PARA}$, IPARA=1 executes no change in YO.

IPHASE(NPHASE, NSETS), Index of the names of the NPHASE species in the vector PNAME. Determined by the computer from comparison of ANAME with PNAME (LISTP).

IREDO, Index of parameter having least significance.

IREG, Local index.

ISIG, Flag to indicate whether SIGYO at input is an absolute measure (=1) or relative measure (=0) of the precision of the value of YO.

ISING, Flag to indicate singularity was found by MINV20, the matrix inverter.

ISTATE(NPHASE, NSETS), If the species is a reference species, set to 1, if the species is an ion or $\text{H}_2\text{O}(\text{liq})$ set to -1, otherwise set to 0.

ISTAY, Flag generated in TEST20 to indicate that at least one parameter has a percent change from the previous cycle greater than 1×10^{-6} .

ISTOP, Flag generated in TEST20 to indicate that all changes in parameters from those of the previous cycle are less than 1×10^{-6} percent. Refinement will terminate.

NAME(MINIMUM DIMENSION), Definition or description

ITFACT, Flag to indicate that the independent variables should be edited: $X(J,I) = X(J,I) + TFACT$.

IW, Flag: options for weighting; 0 for user supplied weights, 1 for weights uniformly set at 1 percent of observed.

IWRITE, Local flag used in EAFW20 to indicate whether a new data set is being calculated. This permits output of the data set reference.

J, Local variable.

JDFLAG, Flag to indicate whether call to UNIQUE is from ORGLS2 thru EAFW20 (JDFLAG=0) or from another routine (JDFLAG≠0). If from ORGLS2, then the derivatives DC(NP) must be supplied in addition to YC.

JN, Local index. Just before the call to ORGLS2, JN is set to zero and becomes JDFLAG in COMMON or in the arguments of the subroutines.

JO, Local index.

K, Local index.

KI(NP), Flag to indicate whether parameters are to refined (KI(I)=1), or held constant (KI(I)=0).

KINVER, Local index.

KO, Local index.

KOUNT, Local index.

L, Local index.

LABEL(NL), LOGICAL*1 Variable containing the alphanumeric legend for the ordinate of the printer plots.

LAST, Local index

LISTP, The number of species in the vector PNAME. Limit is set at 20.

LL, Local index.

LLL, Local index.

LST, Local index.

LSTINV, Local index.

LSTPHA, Local index.

M, Local index.

NC, The number of refinement cycles to be taken by ORGLS2. Generally set to 2 or 3.

NDATA, The number of items in a data set.

NHL, The number of horizontal lines on the printer plot less 1.

NHOLD, The number of parameters to be forced to remain in the regression without regard to the results of TEST20.

NINVER(NPHASE,NSETS), The number of phase transitions which occur in the chemical component between the temperature of the observation $X(1,I)$ and the reference temperature for the elements at 298.15K.

NL, The number of characters in the legend LABEL.

NO, The total number of observations in the problem. Limit is 1200 observations total.

NOYES, Local index.

NP, The numbers of parameters. The limit is set at 140.

NPHAS, Local index.

NPHASE(NSETS), The number of species in the jth set of data.

NREG, The number of problems in the computer run. No limit.

NAME(MINIMUM DIMENSION), Definition or description

NSBH, The number of spaces between the horizontal lines plus 1 on the printer plot.

NSBV, The number of spaces between vertical lines plus 1 on the printer plot.

NSCALE(5), Arguments used to set up the image by the routine PRPLOT. Here all values are set to zero.

NSETS, The numbers of data sets in a problem. Limit is 70 data sets in a problem.

NP, The number of parameters being varied (i.e., KI(I)=1).

NX, The number of independent variables. Limit set at 2.

ONE, The constant 1.0D0.

ORGLS2, Revision of the program OR GLS by Busing and Levy (1962) designed for the peculiar needs of PHAS20.

P(LISTP*7), Parameters for the species.

PARA, Input variable used in editing the dependent variable YO.

PD(NV), Calculated parameter changes for those parameters which are changed.

PHINV(NINVER+1), 8-character alphanumeric labels for each phase in inversion sequence. Begin with the phase stablest 298.15K and progress to include the phase stable at the temperature of observation.

PLOT1, ENTRY points into the routine PRPLOT.

PLOT2

PLOT3

PLOT4

PNAME(LISTP), 8-character alphanumeric labels for each species in the problem.

PUTOUT, Routine called at plot time to calculate the complete set of constants, including "d_i" if constraints are applicable.

R, The gas constant (8.3142 J mol⁻¹K⁻¹) times ln(10) = 19.144379D0.

REF(10,NSETS), 80 character alphanumeric label for each data set.

RELERR, Local variable giving the percent error of each calculated value relative to the observed data.

SC, Local variable containing the stoichiometric variable.

SCINV(2), Constants: -1.0D0, +1.0D0.

SERR(3), The 3 sums-of-errors for a data set.

SERRSQ(3), The 3 sums-of-errors-squared for a data set.

SGN(2), Local variable used during the calculation of "d_i" which is derived from the other parameters because of constraints.

SIGYO(NO), The standard error of an observation YO(I). The reciprocal is used as the weight.

SIX, The constant 6.0D0.

STCOEF(10), Vector of possible stoichiometric coefficients for a change in stoichiometry at a phase transformation. Refer to INVSC above.

STDEV(3), The standard error of the data about the mean error EBAR for a data set.

T, Local variable.

NAME(MINIMUM DIMENSION), Definition or description

TEST20, Routine which does the following: 1) Signals the end of refinement cycling if the percent change in a parameter is less than 10^{-6} , 2) Locates the least significant parameter being refined but not constrained by IHOLD to stay in step-backward elimination, 3) Signals the end of step-backward elimination if the error on all parameters is less than 10 percent.

TFACT, Local input variable used in editing X(J,I) by addition.

THETA, The constant θ of the equation for the dielectric constant of water.

THREE, The constant 3.0D0.

TINV(NPHASE,NSETS,NINVER), The inversion temperatures beginning with the closest temperature to 298.15K.

TITLE(20), 80 character alphanumeric label for the problem.

TK(19,2), Array of temperatures used to calculate the preliminary tables of thermodynamic constants for a species.

TO, Local variable.

TREF, The constant 298.15 which is the reference temperature from the reference state convention.

TWO, The constant 2.0D0.

TYPE, Legends for output of data type.

UNIQUE, Subroutine to be programmed by user if data not considered on Table 1 are available and used in refinement. Refer to Use of the Subroutine UNIQUE.

UNITS, 8 character alphanumeric label for the type of energy data consistent with R and F. As supplied, UNITS has the label 'JOULES'.

VAL(7), Local variables.

X(2,NO), The independent variable. X(1,NO) is the absolute temperature. X(2,NO) is an optional second independent variable used in the current code for the reference temperature of relative heat content data.

XI(1), REAL*4 variable containing the x-coordinate of the datum being passed to the routine PRPLOT.

XMIN, The lowest temperature for the error plot.

XMAX, The highest temperature for the error plot.

YC, The value of the dependent variable calculated from the current set of parameters.

YDERIV, Routine which calculates the temperature-dependent part of the derivative dYC/dP_i .

YESNO(2), The labels 'YES' and 'NO' used in printing input data.

YMAX, The upper bound of the y-axis on the error plot. YMAX= -YMIN.

YMIN, The lower bound of the y-axis on the error plot. YMIN= -YMAX.

YO(NO), The dependent variable.

ZERO, The constant 0.0D0.

ACKNOWLEDGEMENTS

The author thanks James R. Fisher, U.S. Geological Survey, for his patience as the "devil's advocate" during the conception and development of the mathematical model and its use in multiple regression.

Thanks are also due to Blair F. Jones and Al. H. Truesdell, U.S. Geological Survey, who critically read the manuscript and offered valuable suggestions. The project was made possible primarily by support from the Defense Advanced Research Project Agency, Department of Defense (A.R.P.A. Order 1813). Additional support and services were supplied by the Geological Survey and the Office of Saline Water, both of the Department of Interior under O.S.W. Agreement Number 14-30-3040.

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ATTACHMENT A
Example of the Use of the Subroutine UNIQUE

In the text, there is a discussion of the use of the Subroutine UNIQUE with the System Sulfur given as an example. The attached routines UNIQUE, VPRESS, and KJCALC will provide values for YC and DC(NP) for an IGO of 8.

The subroutine UNIQUE calls the appropriate subroutine VPRESS when IGO for the data set is 8. If IGO of the data set is 9, 10, 11 or 12, subroutines SNCOEF, ACTSUL, INFLO, and ININT are called. These are not given, but would contain other constraints on the parameters for the gaseous species in the System Sulfur.

The subroutine KJCALC is a modified version of EAFW20 and returns the eight constants KJ for reaction 16 of the text. KJCALC also generates the data for the matrix TDC(8,NP), the derivatives of each equilibrium constant with respect to the NP parameters of the vector P.

The subroutine VPRESS calculates YC and DN(NP) by summing KJ(8) and TDC(8,NP) for the eight reactions.

SUBROUTINE UNIQUE (YC,N,JO,JDFLAG)	UNI 10
IMPLICIT REAL*8(A-H,C-Z)	UNI 20
DIMENSION COEF(6,70),PNAME(20),TINV(6,70,4),IPHASE(6,70),	UNI 30
1 NPHASE(70),IKCUNT(70),IGU(70),ISTATE(6,70),NINVER(6,70),	UNI 40
2 INSTAT(6,70),INVPH(6,70,5),INVSC(6,70)	UNI 50
COMMON /EAKTH/ CCEF,PNAME,TINV,IPHASE,NPHASE,IKCUNT,IGC,NSFTS,	UNI 60
1 ISTATE,NINVER,INSTAT,INVPH,INVSC,LISTP	UNI 70
M=IGC(JO)-7	UNI 80
GO TO (100,200,300,400,500), M	UNI 90
100 CONTINUE	UNI 100
CALL VPRESS (YC,N,JO,JDFLAG)	UNI 110
RETURN	UNI 120
200 CONTINUE	UNI 130
CALL SDCDEF (YC,N,JO,JDFLAG)	UNI 140
RETURN	UNI 150
300 CONTINUE	UNI 160
CALL ACTSLL (YC,N,JO,JDFLAG)	UNI 170
RETURN	UNI 180
400 CONTINUE	UNI 190
CALL INFLC (YC,N,JO,JDFLAG)	UNI 200
RETURN	UNI 210
500 CONTINUE	UNI 220
CALL ININT (YC,N,JO,JDFLAG)	UNI 230
RETURN	UNI 240
END	UNI 250-

SUBROUTINE VPRESS (YC,I,JO,JCFLAG)	VPR 10
IMPLICIT REAL*8(A-H,C-Z)	VPR 20
REAL*4 TITLE(20)	VPR 30
REAL*8 LOGK(8),KJ(8)	VPR 40
DIMENSION TDC(8,140)	VPR 50
DIMENSION X(2,1200),YC(1200),SIGYC(1200),P(140),KI(140),	VPR 60
1 DC(140),PC(140)	VPR 70
COMMON /AIR/ X, P, DC, TITLE, YG, SIGYC, FC, KI, AC, NV, NX, IW,	VPR 80
I NP, NO, ISING, ISTEP, IL	VPR 90
COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, F	VPR 100
COMMON /BPIM/LOGK,KJ,TDC	VPR 110
YC=ZERO	VPR 120
T=X(1,1)	VPR 130
CALL KJCALC (T,JO)	VPR 140
DO 100 J=2,8	VPR 150
YC=YC+KJ(J)	VPR 160
100 CONTINUE	VPR 170
IF (JCFLAG.NE.0) RETURN	VPR 180
DO 200 K=1,NP	VPR 190
DO 200 J=2,8	VPR 200
DC(K)=DC(K)+TDC(J,K)	VPR 210
200 CONTINUE	VPR 220
RETURN	VPR 230
END	VPR 240-

SLROUTINE KJCALC (T,J)	KJC 10
1 MFLIC(T REAL*8(A=F,C=Z)	KJC 20
0(MENS(CN SGN(2),CC(140)	KJC 30
0(MENS(CN COEF(6,70),PNAME(20),TINV(6,70,4),1PHASE(6,70),	KJC 40
1 NPHASE(70),IKCUNT(70),IGC(70),ISTATE(6,70),NINVER(6,70),	KJC 50
2 ISTAT(6,70),INVPH(6,70,5),INVSC(6,70)	KJC 60
REAL*4 TITLE(20)	KJC 70
DIMENSION X(2,1200),YC(1200),SIGYD(1200),F(140),KI(140),	KJC 80
1 ZZ(140),PD(140)	KJC 90
DIMENSION PFF(10,70),ERRP(140)	KJC 100
DIMENSION DCCC(7),DYCC(7)	KJC 110
DIMENSION SCINV(2),STCOFF(10)	KJC 120
REAL*8 LOGK(8),KJ(8)	KJC 130
DIMENSION TDC(8,140)	KJC 140
COMMON /EARTH/ COEF,PNAME,TINV,IPHASE,NPHASE,IKCUNT,IGC,NSETS,	KJC 150
1 ISTATE,NINVER,ISTAT,INVPH,INVSC,LISTP	KJC 160
COMMON /AIR/ X, P, ZZ, TITLE, YC, SIGYD, FC, KI, NC, NV, NX, IW,	KJC 170
1 AP, N0, ISING, ISTOP, IL, JCFLAG	KJC 180
COMMON /PIPE/ REF, ERRP, IWP(TC, ICY, IICY, IPREC	KJC 190
COMMON /WATER/ZERC, ONE, TWO, THREE, FOUR, SIX, R, F,	KJC 200
1 SCINV, TREF, STCOFF	KJC 210
COMMON /SPACE/ DCCC, DYCC, SC, TC	KJC 220
COMMON /BRIN/LOGK,KJ,TDC	KJC 230
COMMON /WCMAN/LNIG,LCGE	KJC 240
CALL OVERIV (T,5)	KJC 250
IF (IGC(J).NE.12) GO TO 100	KJC 260
M1=IPHASE(3,J)	KJC 270
M2=IPHASE(3,J)	KJC 280
GO TO 200	KJC 290
100 CONTINUE	KJC 300
M1=2	KJC 310
M2=8	KJC 320
200 CONTINUE	KJC 330
DO 1800 M=M1,M2	KJC 340
DO 300 K=1,AP	KJC 350
DC(K)=ZERC	KJC 360
TCC(M,K)=ZERO	KJC 370
300 CONTINUE	KJC 380
LOGK(M)=ZERO	KJC 390
NTEMP=IPHASE(J)	KJC 400
NPHASE(J)=2	KJC 410
IPHASE(2,J)=M	KJC 420
COFF(1,J)=M	KJC 430
COEF(2,J)=1	KJC 440
ISTATE(2,J)=0	KJC 450
NINVER(2,J)=0	KJC 460
LAST=NPHASE(J)	KJC 470
DO 1500 L=1,LAST	KJC 480
INDEX=1+7*(IPHASE(L,J)-1)	KJC 490
SC=COEF(L,J)	KJC 500
IF (ISTATE(L,J).NE.1) GO TO 500	KJC 510
CALL OVERIV (TREF)	KJC 520
DO 400 K=1,7	KJC 530
DC(K+INDEX-1)=DC(K+INDEX-1)+SC*DCCC(K)*DYCC(4)	KJC 540
400 CONTINUE	KJC 550
GO TO 1300	KJC 560
500 CONTINUE	KJC 570
IF (NINVER(L,J).LE.0) GO TO 1300	KJC 580
DO 600 LLL=1,2	KJC 590
SGN(LLL)=SCINV(LLL)	KJC 600

600	CONTINUE	KJC 610
	IF (INVSC(L,J).EQ.0) GO TO 700	KJC 620
	SGN(1)=SGN(1)*STCCFF(INVSC(L,J))	KJC 630
	SGN(2)=SGN(2)*STCCFF(INVSC(L,J))	KJC 640
700	CONTINUE	KJC 650
	IF (INSTAT(L,J).EQ.0) GO TO 900	KJC 660
	IINVR=1+7*(INVPH(L,J,1)-1)	KJC 670
	CALL DDERIV (TREF)	KJC 680
	DO 300 K=1,7	KJC 690
	OC(K+IINVR-1)=OC(K+IINVR-1)+DDOC(K)*SGN(2)*SC*DYDC(4)	KJC 700
800	CONTINUE	KJC 710
900	CONTINUE	KJC 720
	LSTINV=MINVER(L,J)	KJC 730
	DO 1200 LL=1,LSTINV	KJC 740
	CALL DDERIV (TINV(L,J,LL))	KJC 750
	IF (INVSC(L,J).EQ.0) GO TO 1000	KJC 760
	IF (LL.NE.LSTINV) GO TO 1000	KJC 770
	SGN(2)=SGN(2)/STCCFF(INVSC(L,J))	KJC 780
1000	CONTINUE	KJC 790
	DO 1100 LLL=1,2	KJC 800
	IINVR=1+7*(INVPH(L,J,(LL*LLL-1))-1)	KJC 810
	DO 1100 K=1,7	KJC 820
	OC(K+IINVR-1)=OC(K+IINVR-1)+DDOC(K)*SGN(LLL)*SC*DYDC(4)	KJC 830
1100	CONTINUE	KJC 840
1200	CONTINUE	KJC 850
1300	CONTINUE	KJC 860
	DO 1400 K=1,7	KJC 870
	OC(K+INDEX-1)=OC(K+INDEX-1)+SC*CYDC(K)	KJC 880
1400	CONTINUE	KJC 890
1500	CONTINUE	KJC 900
	DO 1600 K=1,NP	KJC 910
	LOGK(M)=LOGK(M)+P(K)*OC(K)	KJC 920
1600	CONTINUE	KJC 930
	IF (LOGK(M).GT.7.5859E1) GO TO 1900	KJC 940
	KJ(4)=1.0E1+LOGK(M)	KJC 950
	OC 1700 K=1,NP	KJC 960
	TDC(M,K)=TDC(M,K)+KJ(M)*LN10*OC(K)	KJC 970
1700	CONTINUE	KJC 980
1800	CONTINUE	KJC 990
	NPHASE(J)=NTEMP	KJC1000
	COEF(1,J)=CNE	KJC1010
	RETURN	KJC1020
1900	CONTINUE	KJC1030
	WRITE (6,2000) M,LOGK(M)	KJC1040
	STOP	KJC1050
2000	FORMAT ('CFOR YOLF',I2,'-TH SPECIES, YOU HAVE TRIED TO CALCULATE	KJC1060
	10.0**',D12.5,'.'/' I JUST CANNOT HACK SUCH LARGE NUMBERS. IT IS	KJC1070
	ZIRING ON THE BRAIN.')	KJC1080
	END	KJC1090-

ATTACHMENT B

EXAMPLES OF AN EXECUTION OF PHAS20

Problem 1.	The System H_2O and the self-ionization of water. . . .	37
Problem 2.	The System Ni-O and the thermodynamics of Bunsenite (NiO).	79

Problem 1. The System H₂O and the self-ionization of water

Consider the System H₂O including the self-ionization of liquid H₂O(water). There are four species:

- H₂O(ideal gas)
- H₂O(liquid, i.e. water)
- H⁺(aqueous hydrated ion)
- OH⁻(aqueous hydrated ion)

In considering this chemical system, the constants for H₂O(ideal gas) are based upon an earlier run and are not further refined here; the constants for H₂O(liquid), H⁺(aq), and OH⁻(aq) are sought. Only the following portion of the data available are used in the refinement to keep the problem in manageable bounds for publication:

1. The equilibrium constant reaction $\text{H}_2\text{O}(\text{liquid}) = \text{H}_2\text{O}(\text{ideal gas})$.
2. The relative heat content data for liquid H₂O.
3. ΔC_p for the self-ionization of liquid H₂O.
4. ΔH for the self-ionization of liquid H₂O.
5. Selected equilibrium constants for the self-ionization of liquid H₂O.

The following pages give the listing of the input and output for the regression of the model to these data.

Listing of input deck. The next four pages contain a listing of the input deck. Deleted from the input are the constants for H₂O(G) which were in the format (7A8).

10/31/73

1
PROBLEM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

1 3 0 1 1
4 C 0
H2O (G) H2O (L) H+ OH-
0-1-1-1

6
H2O(L) = H2O(G), LOG K. HAAS, 1970

2	36	5	0	1	1	0	0
H2O (G)	1.0000	00				0	0
H2O (L)	-1.0000	00				-1	0
0.0100	00	273.1500	00	-2.219700	00	0.008000	00
10.0000	00	273.1500	00	-1.917200	00	0.004000	00
20.0000	00	273.1500	00	-1.637600	00	0.004000	00
30.0000	00	273.1500	00	-1.378800	00	0.004000	00
40.0000	00	273.1500	00	-1.139000	00	0.004000	00
50.0000	00	273.1500	00	-0.916100	00	0.004000	00
60.0000	00	273.1500	00	-0.708500	00	0.004000	00
70.0000	00	273.1500	00	-0.515000	00	0.004000	00
80.0000	00	273.1500	00	-0.334100	00	0.004000	00
90.0000	00	273.1500	00	-0.164900	00	0.004000	00
100.0000	00	273.1500	00	-0.006300	00	0.004000	00
110.0000	00	273.1500	00	0.142400	00	0.005000	00
120.0000	00	273.1500	00	0.282200	00	0.006000	00
130.0000	00	273.1500	00	0.413800	00	0.007000	00
140.0000	00	273.1500	00	0.537600	00	0.008000	00
150.0000	00	273.1500	00	0.654400	00	0.009000	00
160.0000	00	273.1500	00	0.764700	00	0.010000	00
170.0000	00	273.1500	00	0.868900	00	0.011000	00
180.0000	00	273.1500	00	0.967400	00	0.012000	00
190.0000	00	273.1500	00	1.060600	00	0.012000	00
200.0000	00	273.1500	00	1.148900	00	0.013000	00
210.0000	00	273.1500	00	1.232700	00	0.014000	00
220.0000	00	273.1500	00	1.312200	00	0.015000	00
230.0000	00	273.1500	00	1.388600	00	0.015000	00
240.0000	00	273.1500	00	1.459400	00	0.016000	00
250.0000	00	273.1500	00	1.527600	00	0.016000	00
260.0000	00	273.1500	00	1.586000	00	0.017000	00
270.0000	00	273.1500	00	1.654200	00	0.017000	00
280.0000	00	273.1500	00	1.713100	00	0.018000	00
290.0000	00	273.1500	00	1.768200	00	0.018000	00
300.0000	00	273.1500	00	1.822700	00	0.019000	00
310.0000	00	273.1500	00	1.873800	00	0.019000	00
320.0000	00	273.1500	00	1.922700	00	0.019000	00
330.0000	00	273.1500	00	1.969400	00	0.020000	00
340.0000	00	273.1500	00	2.014900	00	0.020000	00
350.0000	00	273.1500	00	2.057000	00	0.020000	00

H2O (L), H(T)-H(273.16) OSBORNE, STIMSON, AND GINNINGS, 1939

2	73	7	0	0	0	-1	0
H2O (L)	1.0000	00				-1	0
H2O (L)	-1.0000	00				-1	0
5.0000	00	273.1500	00	5.0280	00	1.800660	01 0.000500 00 0.010000 00
10.0000	00	273.1500	00	10.0400	00	1.800660	01 0.000500 00 0.010000 00
15.0000	00	273.1500	00	15.0430	00	1.800660	01 0.000500 00 0.010000 00
20.0000	00	273.1500	00	20.0400	00	1.800660	01 0.000500 00 0.010000 00
25.0000	00	273.1500	00	25.0330	00	1.800660	01 0.000500 00 0.010000 00
30.0000	00	273.1500	00	30.0240	00	1.800660	01 0.000500 00 0.010000 00
35.0000	00	273.1500	00	35.0150	00	1.800660	01 0.000500 00 0.010000 00
40.0000	00	273.1500	00	40.0060	00	1.800660	01 0.000500 00 0.010000 00

47.0000	00	273.1500	00	44.9970	00	1.800660	01	0.000500	00	0.010000	00
50.0000	00	273.1500	00	44.9900	00	1.800660	01	0.000500	00	0.010000	00
55.0000	00	273.1500	00	54.9840	00	1.800660	01	0.000500	00	0.010000	00
60.0000	00	273.1500	00	59.9810	00	1.800660	01	0.000500	00	0.010000	00
65.0000	00	273.1500	00	64.9810	00	1.800660	01	0.000500	00	0.010000	00
70.0000	00	273.1500	00	69.9840	00	1.800660	01	0.000500	00	0.010000	00
75.0000	00	273.1500	00	74.9910	00	1.800660	01	0.000500	00	0.010000	00
80.0000	00	273.1500	00	80.0020	00	1.800660	01	0.000500	00	0.010000	00
85.0000	00	273.1500	00	85.0180	00	1.800660	01	0.000500	00	0.010000	00
90.0000	00	273.1500	00	90.0390	00	1.800660	01	0.000500	00	0.010000	00
95.0000	00	273.1500	00	95.0670	00	1.800660	01	0.000500	00	0.010000	00
100.0000	00	273.1500	00	100.1020	00	1.800660	01	0.000500	00	0.010000	00
105.0000	00	273.1500	00	105.1400	00	1.800660	01	0.000500	00	0.010000	00
110.0000	00	273.1500	00	110.1900	00	1.800660	01	0.000500	00	0.010000	00
115.0000	00	273.1500	00	115.2500	00	1.800660	01	0.000500	00	0.010000	00
120.0000	00	273.1500	00	120.3200	00	1.800660	01	0.000500	00	0.010000	00
125.0000	00	273.1500	00	125.4000	00	1.800660	01	0.000500	00	0.010000	00
130.0000	00	273.1500	00	130.4900	00	1.800660	01	0.000500	00	0.010000	00
135.0000	00	273.1500	00	135.6000	00	1.800660	01	0.000500	00	0.010000	00
140.0000	00	273.1500	00	140.7200	00	1.800660	01	0.000500	00	0.010000	00
145.0000	00	273.1500	00	145.8500	00	1.800660	01	0.000500	00	0.010000	00
150.0000	00	273.1500	00	151.0000	00	1.800660	01	0.000500	00	0.010000	00
155.0000	00	273.1500	00	156.1600	00	1.800660	01	0.000500	00	0.010000	00
160.0000	00	273.1500	00	161.3400	00	1.800660	01	0.000500	00	0.010000	00
165.0000	00	273.1500	00	166.5500	00	1.800660	01	0.000500	00	0.010000	00
170.0000	00	273.1500	00	171.7700	00	1.800660	01	0.000500	00	0.010000	00
175.0000	00	273.1500	00	177.0100	00	1.800660	01	0.000500	00	0.010000	00
180.0000	00	273.1500	00	182.2800	00	1.800660	01	0.000500	00	0.010000	00
185.0000	00	273.1500	00	187.5700	00	1.800660	01	0.000500	00	0.010000	00
190.0000	00	273.1500	00	192.8800	00	1.800660	01	0.000500	00	0.010000	00
195.0000	00	273.1500	00	198.2300	00	1.800660	01	0.000500	00	0.010000	00
200.0000	00	273.1500	00	203.5900	00	1.800660	01	0.000500	00	0.010000	00
205.0000	00	273.1500	00	209.0000	00	1.800660	01	0.000500	00	0.010000	00
210.0000	00	273.1500	00	214.4300	00	1.800660	01	0.000500	00	0.010000	00
215.0000	00	273.1500	00	219.9000	00	1.800660	01	0.000500	00	0.010000	00
220.0000	00	273.1500	00	225.4000	00	1.800660	01	0.000500	00	0.010000	00
225.0000	00	273.1500	00	230.9500	00	1.800660	01	0.000500	00	0.010000	00
230.0000	00	273.1500	00	236.5300	00	1.800660	01	0.000500	00	0.010000	00
235.0000	00	273.1500	00	242.1600	00	1.800660	01	0.000500	00	0.010000	00
240.0000	00	273.1500	00	247.8400	00	1.800660	01	0.000500	00	0.010000	00
245.0000	00	273.1500	00	253.5700	00	1.800660	01	0.000500	00	0.010000	00
250.0000	00	273.1500	00	259.3500	00	1.800660	01	0.000500	00	0.010000	00
255.0000	00	273.1500	00	265.1900	00	1.800660	01	0.000500	00	0.010000	00
260.0000	00	273.1500	00	271.0900	00	1.800660	01	0.000500	00	0.010000	00
265.0000	00	273.1500	00	277.0600	00	1.800660	01	0.000500	00	0.010000	00
270.0000	00	273.1500	00	283.0900	00	1.800660	01	0.000500	00	0.010000	00
275.0000	00	273.1500	00	289.2100	00	1.800660	01	0.000500	00	0.010000	00
280.0000	00	273.1500	00	295.4100	00	1.800660	01	0.000500	00	0.010000	00
285.0000	00	273.1500	00	301.7000	00	1.800660	01	0.000500	00	0.010000	00
290.0000	00	273.1500	00	308.1000	00	1.800660	01	0.000500	00	0.010000	00
295.0000	00	273.1500	00	314.6000	00	1.800660	01	0.000500	00	0.010000	00
300.0000	00	273.1500	00	321.2200	00	1.800660	01	0.000500	00	0.010000	00
305.0000	00	273.1500	00	327.9800	00	1.800660	01	0.000500	00	0.010000	00
310.0000	00	273.1500	00	334.8900	00	1.800660	01	0.000500	00	0.010000	00
315.0000	00	273.1500	00	341.9700	00	1.800660	01	0.000500	00	0.010000	00
320.0000	00	273.1500	00	349.2400	00	1.800660	01	0.000500	00	0.010000	00
325.0000	00	273.1500	00	356.7300	00	1.800660	01	0.000500	00	0.010000	00
330.0000	00	273.1500	00	364.4800	00	1.800660	01	0.000500	00	0.010000	00
335.0000	00	273.1500	00	372.5400	00	1.800660	01	0.000500	00	0.010000	00
340.0000	00	273.1500	00	380.9300	00	1.800660	01	0.000500	00	0.010000	00
345.0000	00	273.1500	00	389.7600	00	1.800660	01	0.000500	00	0.010000	00

350.0000 00 273.1500 00 399.1700 00 1.800660 01 0.000500 00 0.010000 00
 355.0000 00 273.1500 00 409.3600 00 1.800660 01 0.000500 00 0.010000 00
 360.0000 00 273.1500 00 420.7400 00 1.800660 01 0.000500 00 0.010000 00
 365.0000 00 273.1500 00 434.1200 00 1.800660 01 0.000500 00 0.010000 00
 H+ + OH- = H2O(L), DELTA CP, REACTION. ACKERMANN, 1958.

3 4 1 0 1 1
 H2O (L) 1.0000 00 -1 0
 H+ -1.0000 00 -1 0
 OH- -1.0000 00 -1 0
 10.0000 00 273.1500 00 69.20000 00 3.000000 00
 30.0000 00 273.1500 00 50.10000 00 3.000000 00
 50.0000 00 273.1500 00 41.80000 00 3.000000 00
 70.0000 00 273.1500 00 42.30000 00 3.000000 00
 H2O = OH- + H+, HEAT OF VAPORIZATION GLOFSSON AND GLOFSSON, 1973.

3 6 3 1 0 1
 H2O (L) -1.0000 00 -1 0
 H+ 1.0000 00 -1 0
 OH- 1.0000 00 -1 0
 298.1500 00 55.92000 032.3900570-01 0.020000 03
 323.1500 00 50.92000 032.3900570-01 0.020000 03
 347.5500 00 46.67000 032.3900570-01 0.020000 03
 373.5500 00 42.07000 032.3900570-01 0.020000 03
 398.4500 00 37.35000 032.3900570-01 0.020000 03
 417.7500 00 33.45000 032.3900570-01 0.020000 03
 LOG KW SIGNOLO, BREWER, AND HEARN, 1971.

3 24 5 0 1 1
 H2O (L) -1.0000 00 -1 0
 H+ 1.0000 00 -1 0
 OH- 1.0000 00 -1 0
 51.0000 00 273.1500 00-13.24100 00 0.021000 00
 60.9000 00 273.1500 00-12.99190 00 0.021000 00
 70.5000 00 273.1500 00-12.80160 00 0.013000 00
 80.2000 00 273.1500 00-12.64170 00 0.013000 00
 89.9000 00 273.1500 00-12.49000 00 0.028000 00
 99.3000 00 273.1500 00-12.23430 00 0.039000 00
 103.6000 00 273.1500 00-12.07450 00 0.025000 00
 118.0000 00 273.1500 00-11.96640 00 0.014000 00
 127.3000 00 273.1500 00-11.86990 00 0.014000 00
 136.7000 00 273.1500 00-11.76720 00 0.020000 00
 146.0000 00 273.1500 00-11.72030 00 0.024000 00
 155.4000 00 273.1500 00-11.60760 00 0.017000 00
 164.7000 00 273.1500 00-11.54770 00 0.015000 00
 174.2000 00 273.1500 00-11.47280 00 0.008000 00
 183.6000 00 273.1500 00-11.39290 00 0.008000 00
 193.0000 00 273.1500 00-11.33260 00 0.014000 00
 202.5000 00 273.1500 00-11.27900 00 0.008000 00
 212.1000 00 273.1500 00-11.25860 00 0.008000 00
 221.7000 00 273.1500 00-11.22830 00 0.008000 00
 231.4000 00 273.1500 00-11.21550 00 0.008000 00
 241.2000 00 273.1500 00-11.20210 00 0.008000 00
 251.0000 00 273.1500 00-11.19560 00 0.009000 00
 261.0000 00 273.1500 00-11.20300 00 0.009000 00
 271.0000 00 273.1500 00-11.21970 00 0.017000 00
 H2O = OH- + H+, LOG KW. SWEETON, MESMER & BAES, PERS COMM, 1973.

3 7 5 0 1 1
 H2O (L) -1.0000 00 -1 0
 H+ 1.0000 00 -1 0
 OH- 1.0000 00 -1 0
 0.0000 00 273.1500 00-14.94100 00 0.009000 00
 50.0000 00 273.1500 00-13.27200 00 0.006000 00
 100.0000 00 273.1500 00-12.26400 00 0.009000 00

```

150.000 00 273.1500 00-11.64200 00      0.012000 00
200.000 00 273.1500 00-11.30200 00      0.012000 00
250.000 00 273.1500 00-11.19600 00      0.015000 00
300.000 00 273.1500 00-11.30100 00      0.045000 00
(A-FORMATED CONSTANTS FROM RUN ON 10/13/73. NOT LISTED) 10/13/73H20 (G)
2.356790 01-1.728260-02 0.0      -5.769160 04-1.097180 02 5.242220-05H20 (L)
-1.069550 03      H20 (L)
0.0      0.0      0.0      0.0      0.0      0.0      H+
0.0      H+
3.080590 02-3.058170-01-1.398640 07-1.498200 05-1.652590 03 0.0      OH-
0.0      OH-
0000000110111100000001111100
4 10 8 10
673.150 00273.150 00 1.0000 01

```

Printed output. The following pages contain a complete printed output from the execution of PHAS20 using the preceding data deck.

THESE RESULTS WERE OBTAINED IN A RLN ON 10/31/73
PROBLEM 1, THE SYSTLM H2O AND THE SELF-IONIZATION OF WATER.

PHASES CONSIDERED IN THIS REGRESSION ARE AS FOLLOWS---

H2O (G)	H2O (L)	H+	OH-
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10/31/73

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

THE FOLLOWING DATA SETS HAVE BEEN READ IN TC STORAGE:

SET NUMBER REFERENCE

MAAS, 1970

1 H2O(L) = H2O(G), LOG K.

THE NUMBER OF PHASES IS: 2
THE NUMBER OF OBSERVATIONS IS: 36
THE TYPE OF DATA IS: LOG K

INVERSIONS

REF. STATE

COEFFICIENT

PHASE NAME
H2C (G)
H2C (L)

1.000
-1.000

NO
NO

INDEX

12

TEMPERATURE

T1

LOG K

ERROR

1	273.160	-2.219700 00	8.000000-03
2	283.150	-1.917200 00	4.000000-03
3	293.150	-1.637600 00	4.000000-03
4	303.150	-1.378800 00	4.000000-03
5	313.150	-1.139500 00	4.000000-03
6	323.150	-9.161000-01	4.000000-03
7	333.150	-7.045000-01	4.000000-03
8	343.150	-5.150600-01	4.000000-03
9	353.150	-3.341000-01	4.000000-03
10	363.150	-1.649000-01	4.000000-03
11	373.150	-6.300000-03	5.000000-03
12	383.150	1.424000-01	6.000000-03
13	393.150	2.822000-01	7.000000-03
14	403.150	4.138600-01	8.000000-03
15	413.150	5.376000-01	9.000000-03
16	423.150	6.544000-01	1.000000-02
17	433.150	7.647000-01	1.100000-02
18	443.150	8.689000-01	1.200000-02
19	453.150	9.674000-01	1.300000-02
20	463.150	1.060000 00	1.400000-02
21	473.150	1.148900 00	1.500000-02
22	483.150	1.232700 00	1.600000-02
23	493.150	1.312200 00	1.700000-02
24	503.150	1.388600 00	1.800000-02
25	513.150	1.459400 00	1.900000-02
26	523.150	1.527600 00	2.000000-02
27	533.150	1.586000 00	1.700000-02
28	543.150	1.634200 00	1.800000-02
29	553.150	1.671300 00	1.900000-02
30	563.150	1.708200 00	1.900000-02
31	573.150	1.822700 00	1.900000-02
32	583.150	1.873800 00	1.900000-02
33	593.150	1.922700 00	2.000000-02
34	603.150	1.969400 00	2.000000-02

35 613.150 2.01490 00 2.000000-02
 36 623.150 2.05700 00 2.000000-02

OSBORNE, STIMSON, AND GINNINGS, 1939									
2 H2O (L), HT(T)-P(273.16)									
1-# NUMBER OF PHASES IS: 2									
1-# NUMBER OF OBSERVATIONS (S): 73									
1-# TYPE OF DATA IS: HT2-HT1									
PHASE NAME	CUEFF(CIENT	REF. STATE	INVERSIONS		HT2-HT1		ERROR		
M2C (L)	1.000	NO	0						
M2C (L)	-1.000	NO	0						
INDEX	T2	TEMPERATURE	T1						
37	276.150	273.160	273.160	9.053720	01	4.526860-02			
38	282.150	273.160	273.160	1.837860	02	9.039310-02			
39	288.150	273.160	273.160	2.708730	02	1.354370-01			
40	294.150	273.160	273.160	3.608520	02	1.804260-01			
41	298.150	273.160	273.160	4.507590	02	2.253800-01			
42	303.150	273.160	273.160	5.406330	02	2.703150-01			
43	308.150	273.160	273.160	6.305010	02	3.152510-01			
44	313.150	273.160	273.160	7.203720	02	3.601860-01			
45	318.150	273.160	273.160	8.102430	02	4.051210-01			
46	323.150	273.160	273.160	9.001500	02	4.500750-01			
47	328.150	273.160	273.160	9.900750	02	4.950170-01			
48	333.150	273.160	273.160	1.030050	03	5.400270-01			
49	338.150	273.160	273.160	1.170090	03	5.850430-01			
50	343.150	273.160	273.160	1.260170	03	6.300870-01			
51	348.150	273.160	273.160	1.350330	03	6.751660-01			
52	353.150	273.160	273.160	1.440560	03	7.202820-01			
53	358.150	273.160	273.160	1.530890	03	7.654430-01			
54	363.150	273.160	273.160	1.621000	03	8.106480-01			
55	368.150	273.160	273.160	1.711830	03	8.559170-01			
56	373.150	273.160	273.160	1.802500	03	9.012480-01			
57	378.150	273.160	273.160	1.893210	03	9.466070-01			
58	383.150	273.160	273.160	1.984150	03	9.923740-01			
59	388.150	273.160	273.160	2.075260	03	1.037630-00			
60	393.150	273.160	273.160	2.166550	03	1.093290-00			
61	398.150	273.160	273.160	2.258030	03	1.129010-00			
62	403.150	273.160	273.160	2.349680	03	1.174840-00			
63	408.150	273.160	273.160	2.441650	03	1.220850-00			
64	413.150	273.160	273.160	2.533890	03	1.266940-00			
65	418.150	273.160	273.160	2.626260	03	1.313130-00			
66	423.150	273.160	273.160	2.719000	03	1.359500-00			
67	428.150	273.160	273.160	2.811510	03	1.405960-00			
68	433.150	273.160	273.160	2.905180	03	1.452590-00			
69	438.150	273.160	273.160	2.999000	03	1.499500-00			
70	443.150	273.160	273.160	3.092590	03	1.546500-00			
71	448.150	273.160	273.160	3.187350	03	1.593670-00			
72	453.150	273.160	273.160	3.282240	03	1.641120-00			
73	458.150	273.160	273.160	3.377500	03	1.688750-00			
74	463.150	273.160	273.160	3.473110	03	1.736560-00			
75	468.150	273.160	273.160	3.569450	03	1.784720-00			
76	473.150	273.160	273.160	3.665560	03	1.832980-00			

INDEX	PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS	HEAT CAP	ERROR
77	47E.150	273.160			3.763380 03	1.881690 00
78	48E.150	273.160			3.861160 03	1.930580 00
79	49E.150	273.160			3.956650 03	1.975830 00
80	49E.150	273.160			4.058650 03	2.029340 00
81	49E.150	273.160			4.158620 03	2.079310 00
82	50E.150	273.160			4.259100 03	2.125550 00
83	50E.150	273.160			4.360480 03	2.180240 00
84	51E.150	273.160			4.462760 03	2.231380 00
85	51E.150	273.160			4.565920 03	2.282570 00
86	52E.150	273.160			4.670010 03	2.335010 00
87	52E.150	273.160			4.775170 03	2.387590 00
88	53E.150	273.160			4.891410 03	2.440700 00
89	53E.150	273.160			4.968510 03	2.494450 00
90	54E.150	273.160			5.077490 03	2.548740 00
91	54E.150	273.160			5.207690 03	2.613840 00
92	55E.150	273.160			5.319330 03	2.656660 00
93	55E.150	273.160			5.425900 03	2.716300 00
94	56E.150	273.160			5.547830 03	2.773520 00
95	56E.150	273.160			5.664880 03	2.832440 00
96	57E.150	273.160			5.784080 03	2.892040 00
97	57E.150	273.160			5.905800 03	2.952500 00
98	58E.150	273.160			6.030230 03	3.015120 00
99	58E.150	273.160			6.157720 03	3.078660 00
100	59E.150	273.160			6.288620 03	3.144310 00
101	59E.150	273.160			6.423450 03	3.211750 00
102	60E.150	273.160			6.563050 03	3.281520 00
103	60E.150	273.160			6.708180 03	3.354050 00
104	61E.150	273.160			6.855250 03	3.428630 00
105	61E.150	273.160			7.018250 03	3.509130 00
106	62E.150	273.160			7.187690 03	3.583850 00
107	62E.150	273.160			7.371180 03	3.685550 00
108	63E.150	273.160			7.576100 03	3.788050 00
109	63E.150	273.160			7.817030 03	3.908510 00

3 H+ + OH- = H2O(l), DELTA CP, REACTION. ACKERMANN, 1958.

THE NUMBER OF PHASES IS: 3
THE NUMBER OF OBSERVATIONS IS: 4
THE TYPE OF DATA IS: HEAT CAP

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS	HEAT CAP	ERROR
H2C (l)	1.000	NJ	0	6.920000 01	3.000000 00
H+	-1.000	NC	0	5.010000 01	3.000000 00
OH-	-1.000	NO	0	4.180000 01	3.000000 00
				4.230000 01	3.000000 00

H₂O = OH + H, HEAT OF IONIZATION . OLOFSSON AND OLOFSSON, 1973.

4

THE NUMBER OF PHASES IS: 3
THE NUMBER OF OBSERVATIONS IS: 6
THE TYPE OF DATA IS: ENTHALPY

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS	INDEX	T2	TEMPERATURE	T1	ENTHALPY	ERRCR
H ₂ O (L)	-1.000	NO	0	114	298.150		-	1.336520 04	4.780110 00
H ₂ O	1.000	NO	0	115	323.150		-	1.217020 04	4.780110 00
OH	1.000	NO	0	116	347.550		-	1.115440 04	4.780110 00
				117	373.550		-	1.005500 04	4.780110 00
				118	398.450		-	8.926860 03	4.780110 00
				119	417.750		-	7.994740 03	4.780110 00

BIGNOLD, BREWER, AND MEYER, 1971.

5

THE NUMBER OF PHASES IS: 3
THE NUMBER OF OBSERVATIONS IS: 24
THE TYPE OF DATA IS: LCG K

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS	INDEX	T2	TEMPERATURE	T1	LCG K	ERRCR
H ₂ O (L)	-1.000	NO	0	120	324.150		-	-1.324100 01	2.100000-02
H ₂ O	1.000	NO	0	121	334.050		-	-1.299150 01	2.100000-02
OH	1.000	NO	0	122	343.650		-	-1.280160 01	1.300000-02
				123	353.350		-	-1.264170 01	1.000000-02
				124	363.050		-	-1.249000 01	2.800000-02
				125	372.450		-	-1.223430 01	3.900000-02
				126	381.750		-	-1.207450 01	2.500000-02
				127	391.150		-	-1.198640 01	1.400000-02
				128	400.450		-	-1.186950 01	1.400000-02
				129	409.850		-	-1.176720 01	2.000000-02
				130	419.150		-	-1.172680 01	2.400000-02
				131	428.550		-	-1.160760 01	1.700000-02
				132	437.850		-	-1.154770 01	1.500000-02
				133	447.250		-	-1.147280 01	8.000000-03
				134	456.750		-	-1.139250 01	8.000000-03
				135	466.150		-	-1.133260 01	1.400000-02
				136	475.650		-	-1.127900 01	8.000000-03
				137	485.250		-	-1.125860 01	8.000000-03
				138	494.850		-	-1.122830 01	8.000000-03

139	504.550	-	-1.121550 01	8.000000-03
140	514.350	-	-1.120210 01	8.000000-03
141	524.150	-	-1.119560 01	9.000000-03
142	534.150	-	-1.120380 01	9.000000-03
143	544.150	-	-1.121970 01	1.700000-02

6 H2O = OH- + H+ LOG Kw. SWEETON, MESMER & BAES, PERS COMM, 1973.

THE NUMBER OF PHASES IS: 3
 THE NUMBER OF OBSERVATIONS IS: 7
 THE TYPE OF DATA IS: LCG K

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS	LCG K	ERROR
H2C (L)	-1.000	NO	0		
H+	1.000	NO	0		
OH-	1.000	AC	0		
INDEX	T2	TEMPERATURE	T1		
144	273.150		-	-1.494100 01	9.000000-03
145	323.150		-	-1.327200 01	6.000000-03
146	373.150		-	-1.226400 01	5.000000-03
147	423.150		-	-1.164200 01	1.200000-02
148	473.150		-	-1.130200 01	1.200000-02
149	523.150		-	-1.119600 01	1.500000-02
150	573.150		-	-1.130100 01	4.500000-02

THE INDEX OF THE LAST ITEM OF THE ABOVE DATA SETS IN THE VECTORS X(1:1), Y(1:1), AND SIGY(1:1) IS AS FOLLOWS:

DATA SET	INDEX
1	36
2	109
3	112
4	115
5	142
6	150

PROBLEM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

NUMBER OF CYCLES IN THIS JOB IS 3

NUMBER OF PARAMETERS TO BE VARIED IS 11

NUMBER OF INDEPENDENT VARIABLES PER OBSERVATION IS 2

DERIVATIVES PROGRAMMED IN SUBROUTINE EAFH2O.

4 EIGHTS TO BE SUPPLIED BY USER

NUMBER OF PARAMETERS READ IS 28

NUMBER OF OBSERVATIONS READ IS 150

TYPICAL CONSTANTS

1 P(1) K(1)

H2O (G)

1 1.76111 03 0

2 3.28200-03 0

3 -5.33300 04 0

4 -4.51600 04 0

5 4.28800 01 0

6 -1.15000-06 0

7 8.64500 01 0

H2O (L)

8 2.35600 04 1

9 -1.72800-02 1

10 0.0 0

11 -5.76000 04 1

12 -1.05700 02 1

13 5.24200-05 1

14 -1.06900 03 1

H+

15 0.0 0

16 0.0 0

17 0.0 0

18 0.0 0

19 0.0 0

20 0.0 0

21 0.0 0

OH-

22 3.08300 02 1

23 -3.95800-04 1

24 -1.39800 07 1

25 -1.45800 05 1

26 -1.65200 03 1

27 0.0 0

28 0.0 0

PROBLEM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE 1

INDEX	T(2)	T(1)	Y(OBS)	Y(CALC)	OBS-CALC	SIG(1)	(O-C)/SIG(1)
H2O(L) = H2O(L), LOG K.							
1	273.150		-2.2197	-2.2262	0.0065	0.0080	0.8126
2	283.150		-1.9172	-1.9229	0.0057	0.0040	1.4170
3	293.150		-1.6376	-1.6426	0.0050	0.0040	1.2461
4	303.150		-1.3788	-1.3833	0.0045	0.0040	1.1135
5	313.150		-1.1390	-1.1428	0.0038	0.0040	0.9453
6	323.150		-0.9161	-0.9193	0.0032	0.0040	0.8056
7	333.150		-0.7285	-0.7313	0.0028	0.0040	0.7359
8	343.150		-0.5150	-0.5173	0.0023	0.0040	0.5919
9	353.150		-0.3141	-0.3161	0.0020	0.0040	0.5014
10	363.150		-0.1649	-0.1666	0.0017	0.0040	0.4142
11	373.150		-0.0363	-0.0377	0.0014	0.0040	0.3502
12	383.150		0.1424	0.1413	0.0011	0.0040	0.2127
13	393.150		0.2822	0.2813	0.0009	0.0040	0.1441
14	403.150		0.4138	0.4120	0.0008	0.0040	0.1148
15	413.150		0.5376	0.5370	0.0006	0.0040	0.0812
16	423.150		0.6544	0.6538	0.0006	0.0040	0.0707
17	433.150		0.7647	0.7639	0.0008	0.0100	0.0751
18	443.150		0.8689	0.8680	0.0009	0.0110	0.0846
19	453.150		0.9674	0.9662	0.0012	0.0120	0.0869
20	463.150		1.0606	1.0592	0.0014	0.0130	0.1157
21	473.150		1.1489	1.1471	0.0018	0.0140	0.1410
22	483.150		1.2327	1.2303	0.0024	0.0160	0.1735
23	493.150		1.3122	1.3091	0.0031	0.0150	0.2089
24	503.150		1.3886	1.3837	0.0049	0.0150	0.3254
25	513.150		1.4594	1.4545	0.0049	0.0160	0.3085
26	523.150		1.5216	1.5215	0.0001	0.0160	0.1755
27	533.150		1.5860	1.5811	0.0049	0.0170	0.0515
28	543.150		1.6542	1.6454	0.0088	0.0170	0.5205
29	553.150		1.7131	1.7025	0.0106	0.0180	0.5509
30	563.150		1.7682	1.7566	0.0116	0.0180	0.6457
31	573.150		1.8227	1.8078	0.0149	0.0190	0.7837
32	583.150		1.8738	1.8563	0.0175	0.0190	0.9224
33	593.150		1.9227	1.9021	0.0206	0.0190	1.0868
34	603.150		1.9694	1.9452	0.0242	0.0200	1.2059
35	613.150		2.0149	1.9858	0.0291	0.0200	1.4573
36	623.150		2.0570	2.0237	0.0333	0.0200	1.6652

H2O (L), H2O(T)-H(273.16) OS8CRNE, STIMSON, AND GINNINGS, 1939

INDEX	T(2)	T(1)	Y(OBS)	Y(CALC)	OBS-CALC	SIG(1)	(O-C)/SIG(1)
37	278.150	273.160	90.5372	90.2942	0.2430	0.0453	5.3677
38	283.150	273.160	180.7863	180.6458	0.1364	0.0934	1.5052
39	288.150	273.160	270.9730	270.8554	0.1176	0.1354	-0.1538
40	293.150	273.160	360.8521	361.0565	-0.2044	0.1804	-1.1347
41	298.150	273.160	450.7590	451.1360	-0.3770	0.2254	-1.6718
42	303.150	273.160	540.6301	541.1501	-0.5200	0.2703	-1.9243
43	308.150	273.160	630.5010	631.1138	-0.6128	0.3153	-1.9435
44	313.150	273.160	720.3718	721.6400	-0.6682	0.3602	-1.8552
45	318.150	273.160	810.2429	810.5436	-0.3007	0.4051	-1.7255
46	323.150	273.160	900.1499	900.8379	-0.6880	0.4501	-1.5285
47	328.150	273.160	990.0747	990.7368	-0.6621	0.4950	-1.3375
48	333.150	273.160	1080.0537	1080.4550	-0.4013	0.5400	-1.1132
49	338.150	273.160	1170.0867	1170.6060	-0.5192	0.5850	-0.8875
50	343.150	273.160	1260.1738	1260.6042	-0.4305	0.6301	-0.6833

51	348.150	273.160	1350.3328	1350.6641	-0.3313	0.6752	-0.4507
52	353.150	273.160	1440.5640	1440.7593	-0.2359	0.7203	-0.3275
53	358.150	273.160	1530.8850	1531.0256	-0.1407	0.7654	-0.1835
54	363.150	273.160	1621.2961	1621.3564	-0.0604	0.8106	-0.0745
55	368.150	273.160	1711.8333	1711.8065	0.0265	0.8559	-0.0309
56	373.150	273.160	1802.4966	1802.3914	0.1051	0.9012	0.1166
57	378.150	273.160	1893.2159	1893.1252	0.0885	0.9466	0.0935
58	383.150	273.160	1984.1472	1984.0234	0.1237	0.9921	0.1247
59	388.150	273.160	2075.2605	2075.1013	0.1583	1.0376	0.1535
60	393.150	273.160	2166.5540	2166.3740	0.1759	1.0833	0.1641
61	398.150	273.160	2258.0276	2257.8577	0.1697	1.1290	0.1503
62	403.150	273.160	2349.6812	2349.5681	0.1129	1.1748	0.0941
63	408.150	273.160	2441.6948	2441.5217	0.1731	1.2208	0.1418
64	413.150	273.160	2533.8887	2533.7345	0.1538	1.2665	0.1214
65	418.150	273.160	2626.2625	2626.2246	0.0380	1.3131	0.0289
66	423.150	273.160	2718.9966	2719.0081	-0.0116	1.3595	-0.0084
67	428.150	273.160	2811.9106	2812.1035	-0.1930	1.4060	-0.1173
68	433.150	273.160	2905.1848	2905.5291	-0.3444	1.4526	-0.2171
69	438.150	273.160	2998.9993	2999.3040	-0.3048	1.4995	-0.2013
70	443.150	273.160	3092.9937	3093.4475	-0.4539	1.5465	-0.2435
71	448.150	273.160	3187.3481	3187.5805	-0.6323	1.5937	-0.3448
72	453.150	273.160	3282.2429	3282.5241	-0.6812	1.6411	-0.4151
73	458.150	273.160	3377.4578	3378.5008	-0.8029	1.6887	-0.4755
74	463.150	273.160	3473.1128	3474.1340	-1.0212	1.7366	-0.5881
75	468.150	273.160	3569.4482	3570.4490	-1.0007	1.7847	-0.5607
76	473.150	273.160	3665.9636	3667.2717	-1.3081	1.8330	-0.7136
77	478.150	273.160	3763.3794	3764.6304	-1.2512	1.8817	-0.6645
78	483.150	273.160	3861.1550	3862.5554	-1.4003	1.9306	-0.7253
79	488.150	273.160	3959.6511	3961.0751	-1.4278	1.9788	-0.7212
80	493.150	273.160	4058.6875	4060.2363	-1.5489	2.0293	-0.7633
81	498.150	273.160	4158.6211	4160.0625	-1.4415	2.0753	-0.6433
82	503.150	273.160	4259.0977	4260.6055	-1.5074	2.1295	-0.7079
83	508.150	273.160	4360.4766	4361.9102	-1.4323	2.1902	-0.6565
84	513.150	273.160	4462.7539	4464.0155	-1.2666	2.2314	-0.5676
85	518.150	273.160	4565.9297	4566.5961	-1.0662	2.2830	-0.4670
86	523.150	273.160	4670.0378	4670.5022	-0.8936	2.3350	-0.3527
87	528.150	273.160	4775.1680	4775.6086	-0.6385	2.3976	-0.2274
88	533.150	273.160	4881.4063	4881.7852	-0.3795	2.4607	-0.1555
89	538.150	273.160	4988.9363	4988.9236	-0.0254	2.4945	-0.0102
90	543.150	273.160	5097.4883	5097.2438	0.1427	2.5487	0.0560
91	548.150	273.160	5207.6875	5207.1367	0.5457	2.6038	0.2111
92	553.150	273.160	5319.3281	5318.4453	0.8834	2.6597	0.3321
93	558.150	273.160	5432.5858	5431.4180	1.1713	2.7163	0.4312
94	563.150	273.160	5547.8329	5546.2344	1.5971	2.7739	0.5758
95	568.150	273.160	5664.8759	5663.0977	1.7753	2.8324	0.6268
96	573.150	273.160	5784.0781	5782.2539	1.8257	2.8920	0.6313
97	578.150	273.160	5905.8008	5903.5766	1.8262	2.9529	0.6184
98	583.150	273.160	6030.2266	6028.6055	1.6235	3.0151	0.5385
99	588.150	273.160	6157.7148	6156.5352	1.1818	3.0789	0.3834
100	593.150	273.160	6288.6211	6288.2344	0.3850	3.1443	0.1237
101	598.150	273.160	6423.4922	6424.2734	-0.7816	3.2117	-0.2434
102	603.150	273.160	6563.0430	6565.3359	-2.2929	3.2815	-0.6590
103	608.150	273.160	6708.1758	6712.2539	-4.0777	3.3541	-1.2157
104	613.150	273.160	6859.2559	6866.0391	-6.7867	3.4296	-1.9788
105	618.150	273.160	7018.2500	7027.5375	-9.6860	3.5091	-2.7602
106	623.150	273.160	7187.6914	7199.4883	-11.7958	3.5938	-3.2822
107	628.150	273.160	7371.1797	7382.6133	-11.4339	3.6856	-3.1023
108	633.150	273.160	7576.0938	7579.7188	-3.6250	3.7880	-0.9570
109	638.150	273.160	7817.0234	7793.8516	23.1736	3.9085	5.9290

Y + O₂ = H₂O(L), DELTA CP, REACTION. ACKERMANN, 1958.

110 283.150
111 303.150
112 323.150
113 343.150

65.2000
50.1000
41.8000
42.3000

57.6360
47.5468
41.5055
38.6071

11.5660
2.5532
0.2945
3.6929

3.0000
3.0000
3.0000
3.0000

3.8547
0.8511
0.0582
1.2310

114 298.150
115 323.150
116 347.550
117 373.550
118 398.450
119 417.750

132.65.1953
12170.1680
11156.3745
10054.9888
8526.8594
7554.7383

13486.3008
12358.4047
11393.1055
10398.2070
9396.8237
8547.6211

-121.1352
-188.6371
-219.7103
-343.2375
-469.8237
-552.8833

4.7801
4.7801
4.7801
4.7801
4.7801
4.7801

-25.1152
-35.4029
-49.5182
-71.8553
-98.2872
-115.6637

120 324.150
121 344.350
122 363.650
123 383.350
124 403.050
125 422.750
126 442.450
127 462.150
128 481.850
129 501.550
130 521.250
131 540.950
132 560.650
133 580.350
134 600.050
135 619.750
136 639.450
137 659.150
138 678.850
139 698.550
140 718.250
141 737.950
142 757.650
143 777.350

-13.2610
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-12.4903
-12.3443
-12.2045
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-11.8699
-11.7672
-11.6708
-11.5876
-11.5177
-11.4578
-11.3929
-11.3326
-11.2790
-11.2286
-11.1823
-11.1405
-11.1021
-11.0676
-11.0368
-11.0097
-10.9865

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-12.3475
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-11.2873
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-10.8580
-10.8263
-10.8015
-10.7839
-10.7732
-10.7655

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0.0210
0.0130
0.0130
0.0280
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0.0250
0.0140
0.0140
0.0200
0.0240
0.0170
0.0150
0.0080
0.0080
0.0140
0.0080
0.0080
0.0080
0.0080
0.0080
0.0050
0.0090
0.0170

-11.3445
-11.3154
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-11.5614
-5.8926
-8.6321
-18.8771
-15.3686
-14.1256
-14.1254
-18.8415
-22.5465
-43.4573
-42.0352
-24.0267
-42.0110
-45.2341
-46.2845
-48.6516
-50.3710
-45.7412
-47.8459
-26.4845

-25.3772
-40.5505
-30.0644
-25.1150
-28.8165
-27.3732
-11.1883

144 273.150
145 323.150
146 373.150
147 423.150
148 473.150
149 523.150
150 573.150

-14.9410
-13.2120
-12.2640
-11.6420
-11.3020
-11.1960
-11.3010

-0.2284
-0.2435
-0.2706
-0.3016
-0.3458
-0.4106
-0.5035

0.0090
0.0160
0.0390
0.0120
0.0120
0.0150
0.0450

-25.3772
-40.5505
-30.0644
-25.1150
-28.8165
-27.3732
-11.1883

154 273.150
155 323.150
156 373.150
157 423.150
158 473.150
159 523.150
160 573.150

-14.9410
-13.2120
-12.2640
-11.6420
-11.3020
-11.1960
-11.3010

-0.2284
-0.2435
-0.2706
-0.3016
-0.3458
-0.4106
-0.5035

0.0090
0.0160
0.0390
0.0120
0.0120
0.0150
0.0450

-25.3772
-40.5505
-30.0644
-25.1150
-28.8165
-27.3732
-11.1883

164 273.150
165 323.150
166 373.150
167 423.150
168 473.150
169 523.150
170 573.150

-14.9410
-13.2120
-12.2640
-11.6420
-11.3020
-11.1960
-11.3010

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-0.2435
-0.2706
-0.3016
-0.3458
-0.4106
-0.5035

0.0090
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0.0390
0.0120
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-25.3772
-40.5505
-30.0644
-25.1150
-28.8165
-27.3732
-11.1883

174 273.150
175 323.150
176 373.150
177 423.150
178 473.150
179 523.150
180 573.150

-14.9410
-13.2120
-12.2640
-11.6420
-11.3020
-11.1960
-11.3010

-0.2284
-0.2435
-0.2706
-0.3016
-0.3458
-0.4106
-0.5035

0.0090
0.0160
0.0390
0.0120
0.0120
0.0150
0.0450

-25.3772
-40.5505
-30.0644
-25.1150
-28.8165
-27.3732
-11.1883

184 273.150
185 323.150
186 373.150
187 423.150
188 473.150
189 523.150
190 573.150

-14.9410
-13.2120
-12.2640
-11.6420
-11.3020
-11.1960
-11.3010

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-0.2435
-0.2706
-0.3016
-0.3458
-0.4106
-0.5035

0.0090
0.0160
0.0390
0.0120
0.0120
0.0150
0.0450

-25.3772
-40.5505
-30.0644
-25.1150
-28.8165
-27.3732
-11.1883

194 273.150
195 323.150
196 373.150
197 423.150
198 473.150
199 523.150
200 573.150

-14.9410
-13.2120
-12.2640
-11.6420
-11.3020
-11.1960
-11.3010

-0.2284
-0.2435
-0.2706
-0.3016
-0.3458
-0.4106
-0.5035

0.0090
0.0160
0.0390
0.0120
0.0120
0.0150
0.0450

-25.3772
-40.5505
-30.0644
-25.1150
-28.8165
-27.3732
-11.1883

OLCFSSCN AND OLOFSSON, 1973.

BIGNOLO, BREMER, AND MCARN, 1971.

SWEETON, MESMER & BAES, PERS COMM, 1973.

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 1

SUM((10-C)**2) IS 0.6250 05

SCRIPT(SUM((10-C)**2)/(10-NV)) IS 0.21200 02

PROBLEM 1: THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

PARAMETERS AFTER LEAST SQUARES CYCLE 1

	OLD	CHANGE	NEW	ERROR	PCT. CHANGE	PCT. ERROR
P-2C (G)						
1	1.76055830430 00	1.76055830430 C0				
2	3.28246628230-03	3.28246628230-C3				
3	-5.33383252400 04	-5.33383252400 C4				
4	-4.51596304610 04	-4.51596304610 C4				
5	4.28795457410 01	4.28795457410 C1				
6	-1.15001512500-06	-1.15001512500-C6				
7	8.64559293830 01	8.64559293830 C1				
H-2C (L)						
8	2.35677999990 01	2.35677999990 C1				
9	-1.72826999990-02	-1.72826999990-C2				
10	0.0	0.0				
11	-5.76916999990 04	-5.76916999990 C4				
12	-1.09719254110 02	-1.09719254110 C2				
13	5.24229762640-05	5.24229762640-C5				
14	-1.06953757100 03	-1.06953757100 C3				
H+						
15	0.0	0.0				
16	0.0	0.0				
17	0.0	0.0				
18	0.0	0.0				
19	0.0	0.0				
20	0.0	0.0				
21	0.0	0.0				
H-						
22	3.53176542570 C1	3.53176542570 C1				
23	-3.56709827420-01	-3.56709827420-C1				
24	-1.54401176550 C6	-1.54401176550 C6				
25	-1.42281959220 04	-1.42281959220 C4				
26	-2.36935685930 C2	-2.36935685930 C2				
27	0.0	0.0				
28	0.0	0.0				

ESTIMATED ADJUSTMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 1

U*(W*(C-C)*2) IS 0.2220 03

SQRTF(SUM(W*(U-C)*2)/(NC-NV)) IS 0.12620 01

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

CALCULATED Y BASED ON PARAMETERS BEFORE CYCLE 2

INDX	T(2)	T(1)	Y(0BS)	Y(CALC)	OBS-CALC	SIG(C)	(O-C)/SIG(C)
H2O(L) = H2O(G), LOG K.							
1	273.160		-2.2197	-2.2230	0.0033	0.0380	0.4163
2	283.150		-1.9172	-1.9197	0.0025	0.0343	0.6180
3	293.150		-1.6376	-1.6394	0.0018	0.0340	0.4412
4	303.150		-1.3788	-1.3800	0.0012	0.0340	0.3028
5	313.150		-1.1393	-1.1405	0.0005	0.0340	0.1291
6	323.150		-0.9161	-0.9161	-0.0000	0.0340	-0.0120
7	333.150		-0.7085	-0.7080	0.0005	0.0340	-0.1210
8	343.150		-0.5150	-0.5140	0.0010	0.0340	-0.2501
9	353.150		-0.3341	-0.3328	0.0013	0.0340	-0.1164
10	363.150		-0.1649	-0.1622	0.0027	0.0340	-0.4274
11	373.150		0.0063	0.0043	0.0020	0.0340	-0.4561
12	383.150		0.1424	0.1447	-0.0023	0.0350	-0.4679
13	393.150		0.2822	0.2848	-0.0026	0.0363	-0.4260
14	403.150		0.4138	0.4164	-0.0026	0.0370	-0.3764
15	413.150		0.5376	0.5404	-0.0028	0.0380	-0.3506
16	423.150		0.6544	0.6572	-0.0028	0.0390	-0.3149
17	433.150		0.7647	0.7674	-0.0027	0.0400	-0.2734
18	443.150		0.8689	0.8715	-0.0026	0.0410	-0.2238
19	453.150		0.9674	0.9698	-0.0024	0.0420	-0.1571
20	463.150		1.0606	1.0627	-0.0021	0.0430	-0.1147
21	473.150		1.1489	1.1506	-0.0017	0.0440	-0.1118
22	483.150		1.2327	1.2338	-0.0011	0.0450	-0.0809
23	493.150		1.3122	1.3126	-0.0004	0.0460	-0.0255
24	503.150		1.3886	1.3873	0.0013	0.0470	0.0342
25	513.150		1.4594	1.4581	0.0013	0.0480	0.0294
26	523.150		1.5276	1.5251	0.0025	0.0490	0.0150
27	533.150		1.5860	1.5827	0.0033	0.0500	0.0170
28	543.150		1.6342	1.6300	0.0042	0.0510	0.0364
29	553.150		1.6713	1.6661	0.0052	0.0520	0.0379
30	563.150		1.7082	1.7021	0.0061	0.0530	0.0422
31	573.150		1.7447	1.7377	0.0070	0.0540	0.0482
32	583.150		1.7807	1.7727	0.0080	0.0550	0.0552
33	593.150		1.8162	1.8072	0.0090	0.0560	0.0621
34	603.150		1.8512	1.8412	0.0100	0.0570	0.0691
35	613.150		1.8857	1.8747	0.0110	0.0580	0.0761
36	623.150		1.9197	1.9077	0.0120	0.0590	0.0831

H2O (L), H(T)-H(273.16)

CSBECNE, STIMSON, AND GINNINGS, 1939

37	278.150	273.160	50.5372	90.2791	0.2590	0.0453	5.7000
38	283.150	273.160	180.7863	180.6157	0.1665	0.0404	1.8478
39	288.150	273.160	270.8730	270.8542	0.0190	0.1354	0.1400
40	293.150	273.160	360.8521	360.8566	-0.0444	0.1844	-0.0806
41	298.150	273.160	450.7590	451.0005	-0.2414	0.2254	-1.3373
42	303.150	273.160	540.6301	541.0558	-0.4257	0.2702	-1.5856
43	308.150	273.160	630.5010	631.0081	-0.5071	0.3153	-1.6386
44	313.150	273.160	720.3718	720.5194	-0.1476	0.3602	-1.5202
45	318.150	273.160	810.2429	810.6076	-0.3647	0.4051	-1.3943
46	323.150	273.160	900.1499	900.8868	-0.7369	0.4501	-1.6432
47	328.150	273.160	990.0747	990.5708	-0.4961	0.4950	-1.0021
48	333.150	273.160	1080.0537	1080.4736	-0.4200	0.5400	-0.7777
49	338.150	273.160	1170.0867	1170.4097	-0.3229	0.5850	-0.5520
50	343.150	273.160	1260.1738	1260.3528	-0.2191	0.6301	-0.3477

51	348.150	273.160	1350.3328	1350.4375	-C.1047	0.6752	-0.1551
52	353.150	273.160	1440.5640	1440.5581	0.0058	0.7203	C.0681
53	358.150	273.160	1530.8850	1530.7688	0.1161	0.7654	0.1517
54	363.150	273.160	1621.2961	1621.0845	0.2116	0.8106	C.2610
55	368.150	273.160	1711.8333	1711.5192	0.3136	0.8559	C.3664
56	373.150	273.160	1802.4966	1802.0891	C.4074	0.9012	0.4520
57	378.150	273.160	1893.2139	1892.8075	0.4059	0.9466	0.4288
58	383.150	273.160	1984.1472	1983.6955	0.4562	0.9921	0.4866
59	388.150	273.160	2074.7534	2074.2534	0.5070	1.0376	0.5455
60	393.150	273.160	2166.5540	2166.0112	0.5427	1.0833	C.5010
61	398.150	273.160	2258.0276	2257.4757	0.5477	1.1293	0.4852
62	403.150	273.160	2349.6812	2349.1750	0.5060	1.1748	C.4307
63	408.150	273.160	2441.6548	2441.1133	0.5814	1.2208	0.4763
64	413.150	273.160	2533.8887	2533.3113	0.5773	1.2669	0.457
65	418.150	273.160	2626.2625	2625.7855	0.5773	1.3131	0.4320
66	423.150	273.160	2718.9966	2718.5544	0.4422	1.3595	0.3752
67	428.150	273.160	2811.9106	2811.6365	0.2760	1.4060	0.3163
68	433.150	273.160	2905.1848	2905.0495	0.1347	1.4526	0.2565
69	438.150	273.160	2998.9993	2998.8047	0.1045	1.4995	0.1967
70	443.150	273.160	3092.9937	3092.5331	0.0605	1.5465	0.1361
71	448.150	273.160	3187.3481	3187.4505	-0.1027	1.5937	-0.0644
72	453.150	273.160	3282.2429	3282.3154	-0.1364	1.6411	-0.0031
73	458.150	273.160	3377.4978	3377.7410	-0.2431	1.6887	-0.0534
74	463.150	273.160	3473.1128	3473.5551	-0.4462	1.7366	-0.1034
75	468.150	273.160	3568.4482	3568.8886	-0.4105	1.7847	-0.1534
76	473.150	273.160	3665.9636	3666.6663	-0.7028	1.8330	-0.2034
77	478.150	273.160	3763.3754	3764.0100	-0.6107	1.8817	-0.2534
78	483.150	273.160	3861.1550	3861.5159	-0.7647	1.9306	-0.3034
79	488.150	273.160	3955.6511	3960.4282	-0.7771	1.9798	-0.3534
80	493.150	273.160	4058.6875	4055.5706	-0.8020	2.0293	-0.4034
81	498.150	273.160	4158.0211	4159.3828	-0.7604	2.0793	-0.4534
82	503.150	273.160	4255.0977	4255.5102	-0.8112	2.1295	-0.5034
83	508.150	273.160	4360.4766	4361.1523	-0.7205	2.1802	-0.5534
84	513.150	273.160	4462.7539	4463.2930	-0.5401	2.2314	-0.6034
85	518.150	273.160	4565.9297	4566.2578	-0.3246	2.2830	-0.6534
86	523.150	273.160	4673.0078	4670.1484	-0.1369	2.3350	-0.7034
87	528.150	273.160	4775.1680	4775.0352	0.1323	2.3876	-0.7534
88	533.150	273.160	4881.4363	4881.0300	0.4075	2.4407	-0.8034
89	538.150	273.160	4988.9063	4988.1289	0.7767	2.4945	-0.8534
90	543.150	273.160	5097.4083	5096.5273	0.9559	2.5487	-0.9034
91	548.150	273.160	5207.6875	5206.3047	1.3820	2.6039	-0.9534
92	553.150	273.160	5315.3281	5317.5577	1.7308	2.6591	-1.0034
93	558.150	273.160	5432.5858	5430.5547	2.0338	2.7163	-1.0534
94	563.150	273.160	5547.8120	5545.3555	2.2748	2.7739	-1.1034
95	568.150	273.160	5664.8750	5662.5070	2.5680	2.8324	-1.1534
96	573.150	273.160	5784.0781	5781.3438	2.7335	2.8920	-1.2034
97	578.150	273.160	5905.8308	5903.0547	2.7492	2.9521	-1.2534
98	583.150	273.160	6030.2266	6027.6680	2.5615	3.0151	-1.3034
99	588.150	273.160	6157.7148	6155.5781	2.1350	3.0789	-1.3534
100	593.150	273.160	6288.6211	6287.2656	1.3572	3.1443	-1.4034
101	598.150	273.160	6423.4922	6423.2851	0.2017	3.2117	-1.4534
102	603.150	273.160	6563.0430	6564.3358	-1.2955	3.2815	-1.5034
103	608.150	273.160	6708.1758	6711.2422	-3.0641	3.3541	-1.5534
104	613.150	273.160	6859.2539	6865.0117	-5.7580	3.4296	-1.6034
105	618.150	273.160	7018.2500	7026.8945	-8.6423	3.5091	-1.6534
106	623.150	273.160	7187.6914	7198.4257	-10.7369	3.5928	-1.7034
107	628.150	273.160	7371.1797	7381.5351	-10.3555	3.6856	-1.7534
108	633.150	273.160	7576.0938	7578.6289	-2.5358	3.7880	-1.8034
109	638.150	273.160	7817.0234	7792.7461	24.2779	3.9095	-1.8534

M + OH - H2O(1); DELTA CP, REACTION. ACKERMANN, 1958.

11J 283.150 69.2J00 60.5542 8.6057 3.0030 2.9686
 11I 303.150 50.1000 50.6836 0.0164 3.0000 0.0055
 112 323.150 41.8000 44.6627 -2.2627 3.0000 -0.7542
 113 343.150 42.3000 41.5267 0.7733 3.0000 0.2578

114 298.150 13365.1553 13365.4453 -0.2473 4.7801 -0.0517
 115 323.150 12170.1680 12174.6320 -4.6628 4.7801 -0.9755
 116 347.550 11154.3945 11141.7617 12.6304 4.7801 2.6423
 117 373.550 10054.9688 10056.6172 -1.6454 4.7801 -0.2451
 118 398.450 8526.8594 8541.5461 -15.1334 4.7801 -3.1656
 119 417.750 7994.7383 7983.0352 11.7039 4.7801 2.4484

OLCFESSEN AND CLOFSSON, 1973.

LOG KW

BIGNOLD, BREWER, AND HEARN, 1971.

120 324.150 -13.2410 -13.2560 0.0150 0.0210 0.7120
 121 334.050 -12.9419 -13.0178 0.0759 0.0210 1.2321
 122 343.650 -12.8016 -12.8275 0.0359 0.0130 0.4551
 123 353.350 -12.6417 -12.6177 -0.0280 0.0130 -2.8047
 124 363.050 -12.4900 -12.4368 -0.0532 0.0260 -1.9006
 125 372.450 -12.2243 -12.2802 0.0459 0.0390 1.1778
 126 391.750 -12.0745 -12.1386 0.0641 0.0250 2.5655
 127 391.150 -11.9364 -12.0080 0.0216 0.0140 1.5440
 128 400.450 -11.8699 -11.8524 0.0205 0.0140 1.4614
 129 409.850 -11.7672 -11.7824 0.0152 0.0200 0.7425
 130 419.150 -11.7238 -11.6800 -0.0448 0.0240 -1.4607
 131 428.550 -11.6076 -11.5984 0.0052 0.0170 -0.5410
 132 437.850 -11.5477 -11.5211 -0.0266 0.0150 -1.7777
 133 447.350 -11.4728 -11.4513 -0.0215 0.0380 -2.6846
 134 456.750 -11.3929 -11.3911 -0.0018 0.0380 -0.2273
 135 466.150 -11.3326 -11.2952 0.0067 0.0140 0.4768
 136 475.650 -11.2790 -11.2952 0.0162 0.0380 2.0258
 137 485.250 -11.2586 -11.2589 0.0023 0.0300 0.0343
 138 494.850 -11.2285 -11.2306 0.0023 0.0380 0.2814
 139 504.550 -11.2155 -11.2098 -0.0057 0.0380 -0.7266
 140 514.350 -11.2021 -11.1968 -0.0053 0.0380 -0.6618
 141 524.150 -11.1956 -11.1915 -0.0041 0.0380 -0.4561
 142 534.150 -11.2038 -11.1939 -0.0099 0.0390 -1.1036
 143 544.150 -11.2197 -11.2039 -0.0158 0.0170 -0.9266

H2C = CH - H*, LOG KW.

SWEETON, MESMER & BAES, PERS COMM, 1973.

144 273.150 -14.9410 -14.5512 0.0102 0.0390 1.1282
 145 323.150 -13.2720 -13.2813 0.0093 0.0060 1.5512
 146 373.150 -12.2640 -12.2651 0.0051 0.0090 0.6458
 147 423.150 -11.6420 -11.6475 0.0055 0.0120 0.4610
 148 473.150 -11.3020 -11.3060 0.0040 0.0120 0.3342
 149 523.150 -11.1960 -11.1917 -0.0043 0.0150 -0.2875
 150 573.150 -11.3010 -11.2755 -0.0255 0.0450 -0.5669

GREENE FACTORS BASED ON PARAMETERS BEFORE CYCLE 2

LM(W*10-C)**2) IS 0.222C 03

CRFISUM(W*(J-C)**2)/(NC-NV)) IS 0.1262C 01

PROBLEM 1: THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.
PARAMETERS AFTER LEAST SQUARES CYCLE 2

	OLD	CHANGE	NEW	ERROR	PCT. CHANGE	PCT. ERROR
P2C (G)						
1	1.76055830430 J0	1.76055830430 C0				
2	3.28246282300-03	3.28246282300-03				
3	-5.33303252400 C4	-5.33303252400 C4				
4	-4.51558364610 D4	-4.51558364610 C4				
5	4.28795557410 D1	4.28795557410 D1				
6	-1.15001512500-06	-1.15001512500-06				
7	8.64570293830 C1	8.64570293830 C1				
H2C (L)						
8	2.35650074940 D1	2.35650074950 D1		9.57322153630-02	1.92429411840-10	0.4062
9	-1.72825277990-02	-1.72825277990-02		2.67005204560-04	7.41778751610-10	1.3549
10	C.C	0.0				
11	-5.76910546200 D4	-5.76910546200 D4		1.80577877930 D1	9.04757593590-12	0.0013
12	-1.09719294110 D2	-1.09719294110 D2		4.20156321860-01	1.78623330050-10	0.3329
13	5.24225762640-05	5.24225762640-05		7.32333652260-07	6.62838458770-10	1.3370
14	-1.06954775790 D3	-1.06954775790 D3		1.00966720590 D1	-3.42980794220-10	0.5440
H+						
15	C.C	0.0				
16	D.O	0.0				
17	C.C	0.0				
18	U.C	0.0				
19	C.C	0.0				
20	O.C	0.0				
21	O.C	0.0				
H-						
22	3.53170542970 D2	-6.74612468650-07	3.53176542290 D2	1.52755674470 C1	-1.51012818780-07	4.3535
23	-3.56704274200-01	6.26337197240-10	-3.56705826800-01	1.43171686230-02	-1.75587312200-07	4.0137
24	-1.55304117650 D7	2.81157183320-02	-1.55304117370 D7	6.44291205280 D5	-1.80392630560-07	4.1486
25	-1.64348195920 D5	2.40194080520-04	-1.64348155680 D5	5.46930914180 D3	-1.46416776800-07	3.3440
26	-1.88952368590 D3	3.61790738590-06	-1.88952368230 D3	8.26759973230 D1	-1.51471317560-07	4.3755
27	C.C	0.0				
28	C.C	0.0				

ESTIMATE AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 2

SLP((10-C)**2) IS 0.2220 D3

SCRT(SUM((U-C)**2)/(NO-NV)) IS 0.12620 D1

SLROUTINE TEST INDICATES THAT JOB IS TO BE TERMINATED FOR REASON 1

PROBLEM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

CORRELATION MATRIX

1	0.10000 01 -0.99770 00 -0.61630 00 -0.99500 00	0.75010 00	0.98970 00	0.53870-02	0.60900-02	0.60230-02
	0.58450-02					
2	0.0	0.61220 00	0.59170 00 -0.99770 00 -0.76030 00	0.58650-02	-0.54880-02	-0.60720-02
	-0.59150-02					
3	0.0	0.10000 01	0.69080 00 -0.60460 00 -0.44750 00	0.35160-02	-0.32560-02	-0.37310-02
	-0.31640-02					
4	0.0	0.0	0.10000 01	0.57400-02	-0.53340-02	-0.57250-02
	-0.57510-02					
5	0.0	0.0	0.10000 01	0.55730-02	0.60990-02	0.60870-02
	0.55610-02					
6	0.0	0.0	0.10000 01	0.47320-02	0.46760-02	0.47530-02
	0.48220-02					
7	0.0	0.0	0.10000 01	-0.99920 00	-0.99770 00	-0.99520 00
	-0.10000 01					
8	0.0	0.0	0.10000 01	0.99330 00	0.99330 00	0.99700 00
	0.99850 00					
9	0.0	0.0	0.10000 01	0.99330 01	0.99330 01	0.99700 01
	0.99750 00					
10	0.0	0.0	0.10000 01	0.99330 01	0.99330 01	0.99700 01
	0.99950 00					
11	0.0	0.0	0.10000 01	0.99330 01	0.99330 01	0.99700 01
	0.10000 01					

10/31/73

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IGNITION OF WATER.

TEMPERATURE		LOG K		DIFFERENCE		PERCENT		DPS-CALC/SIGMO	
T(2)	T(1)	OBSERVED	CALCULATED						
H2O(1) = H2O(2), LOG K.									
H2O(1) = H2O(2), LOG K.									
273.150	273.150	-2.21970 00	-2.22300 00	C-C022	0.1500	0.1289	0.4163		
283.150	283.150	-1.91720 00	-1.91970 00	C-C025	0.1289	0.1289	0.4163		
293.150	293.150	-1.63740 00	-1.63940 00	C-C018	0.1078	0.1078	0.4163		
303.150	303.150	-1.37880 00	-1.38030 00	C-C012	0.0878	0.0878	0.4163		
313.150	313.150	-1.13950 00	-1.13950 00	C-C005	0.0453	0.0453	0.4163		
323.150	323.150	-9.16100 01	-9.16350 01	C-C000	-0.0052	-0.0052	-0.0120		
333.150	333.150	-7.38530 01	-7.39320 01	C-C005	-0.0083	-0.0083	-0.0120		
343.150	343.150	-5.15000 01	-5.15300 01	C-C010	-0.0030	-0.0030	-0.0120		
353.150	353.150	-3.34100 01	-3.32760 01	C-C013	-0.0016	-0.0016	-0.0120		
363.150	363.150	-1.64500 01	-1.63190 01	C-C017	-0.0031	-0.0031	-0.0120		
373.150	373.150	-6.30000 03	-4.31550 03	C-C020	-31.4555	-31.4555	-0.4961		
383.150	383.150	1.42400 01	1.44740 01	C-C023	-1.6429	-1.6429	-0.4619		
393.150	393.150	2.82200 01	2.84760 01	C-C026	-0.9057	-0.9057	-0.4260		
403.150	403.150	4.13800 01	4.16430 01	C-C026	-0.6367	-0.6367	-0.3764		
413.150	413.150	5.37600 01	5.40400 01	C-C028	-0.5217	-0.5217	-0.3506		
423.150	423.150	6.54400 01	6.57230 01	C-C028	-0.4331	-0.4331	-0.3149		
433.150	433.150	7.64700 01	7.67440 01	C-C027	-0.3577	-0.3577	-0.2735		
443.150	443.150	8.68500 01	8.71470 01	C-C026	-0.2960	-0.2960	-0.2328		
453.150	453.150	9.67400 01	9.69760 01	C-C024	-0.2445	-0.2445	-0.1971		
463.150	463.150	1.06000 00	1.06270 00	C-C021	-0.1976	-0.1976	-0.1747		
473.150	473.150	1.14450 00	1.15040 00	C-C017	-0.1491	-0.1491	-0.1319		
483.150	483.150	1.23270 00	1.23300 00	C-C011	-0.0919	-0.0919	-0.0809		
493.150	493.150	1.31220 00	1.31200 00	C-C004	-0.0022	-0.0022	-0.0295		
503.150	503.150	1.38860 00	1.38730 00	C-C013	0.0091	0.0091	0.0862		
513.150	513.150	1.45540 00	1.45810 00	C-C013	0.0914	0.0914	0.0834		
523.150	523.150	1.52760 00	1.52510 00	C-C025	0.1613	0.1613	0.1540		
533.150	533.150	1.58600 00	1.58870 00	C-C027	-0.1714	-0.1714	-0.1599		
543.150	543.150	1.65420 00	1.64900 00	C-C052	0.3148	0.3148	0.3064		
553.150	553.150	1.71310 00	1.70620 00	C-C070	0.4076	0.4076	0.3879		
563.150	563.150	1.76820 00	1.76020 00	C-C080	0.4501	0.4501	0.4422		
573.150	573.150	1.82270 00	1.81150 00	C-C112	0.6152	0.6152	0.5902		
583.150	583.150	1.87380 00	1.86000 00	C-C138	0.7385	0.7385	0.7283		
593.150	593.150	1.92270 00	1.90580 00	C-C165	0.8815	0.8815	0.8921		
603.150	603.150	1.96540 00	1.94890 00	C-C205	1.0403	1.0403	1.0243		
613.150	613.150	2.01490 00	1.98950 00	C-C254	1.2617	1.2617	1.2711		
623.150	623.150	2.05760 00	2.02740 00	C-C296	1.4376	1.4376	1.4785		

THE ARITHMETIC MEAN OF THE FADORS FOR THIS SET ARE -----

THE STANDARD DEVIATIONS ABOUT THE MEAN ARE -----

THE NUMBER OF OBSERVATIONS IS 36

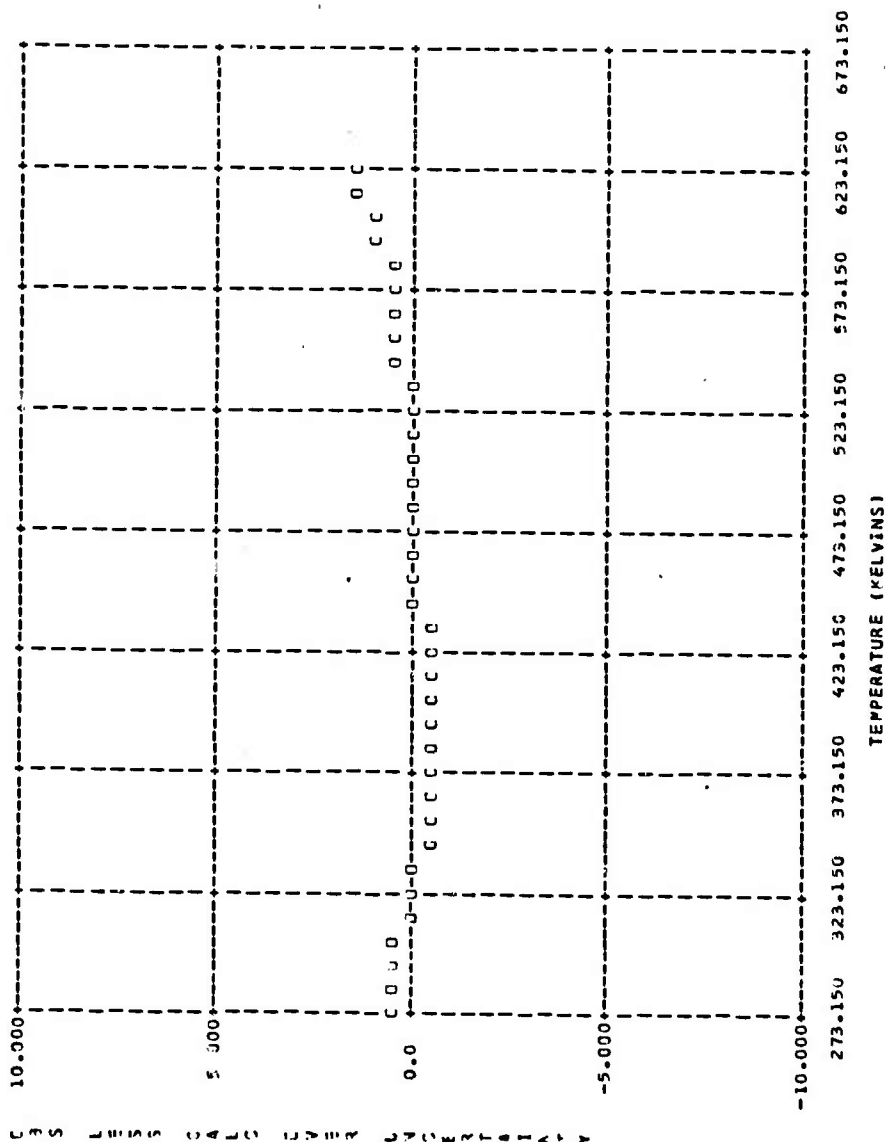
TEMPERATURE		LOG K		DIFFERENCE		PERCENT		DPS-CALC/SIGMO	
T(2)	T(1)	OBSERVED	CALCULATED						
H2O(1) = H2O(2), LOG K.									
H2O(1) = H2O(2), LOG K.									
273.150	273.150	-2.21970 00	-2.22300 00	C-C022	0.1500	0.1289	0.4163		
283.150	283.150	-1.91720 00	-1.91970 00	C-C025	0.1289	0.1289	0.4163		
293.150	293.150	-1.63740 00	-1.63940 00	C-C018	0.1078	0.1078	0.4163		
303.150	303.150	-1.37880 00	-1.38030 00	C-C012	0.0878	0.0878	0.4163		
313.150	313.150	-1.13950 00	-1.13950 00	C-C005	0.0453	0.0453	0.4163		
323.150	323.150	-9.16100 01	-9.16350 01	C-C000	-0.0052	-0.0052	-0.0120		
333.150	333.150	-7.38530 01	-7.39320 01	C-C005	-0.0083	-0.0083	-0.0120		
343.150	343.150	-5.15000 01	-5.15300 01	C-C010	-0.0030	-0.0030	-0.0120		
353.150	353.150	-3.34100 01	-3.32760 01	C-C013	-0.0016	-0.0016	-0.0120		
363.150	363.150	-1.64500 01	-1.63190 01	C-C017	-0.0031	-0.0031	-0.0120		
373.150	373.150	-6.30000 03	-4.31550 03	C-C020	-31.4555	-31.4555	-0.4961		
383.150	383.150	1.42400 01	1.44740 01	C-C023	-1.6429	-1.6429	-0.4619		
393.150	393.150	2.82200 01	2.84760 01	C-C026	-0.9057	-0.9057	-0.4260		
403.150	403.150	4.13800 01	4.16430 01	C-C026	-0.6367	-0.6367	-0.3764		
413.150	413.150	5.37600 01	5.40400 01	C-C028	-0.5217	-0.5217	-0.3506		
423.150	423.150	6.54400 01	6.57230 01	C-C028	-0.4331	-0.4331	-0.3149		
433.150	433.150	7.64700 01	7.67440 01	C-C027	-0.3577	-0.3577	-0.2735		
443.150	443.150	8.68500 01	8.71470 01	C-C026	-0.2960	-0.2960	-0.2328		
453.150	453.150	9.67400 01	9.69760 01	C-C024	-0.2445	-0.2445	-0.1971		
463.150	463.150	1.06000 00	1.06270 00	C-C021	-0.1976	-0.1976	-0.1747		
473.150	473.150	1.14450 00	1.15040 00	C-C017	-0.1491	-0.1491	-0.1319		
483.150	483.150	1.23270 00	1.23300 00	C-C011	-0.0919	-0.0919	-0.0809		
493.150	493.150	1.31220 00	1.31200 00	C-C004	-0.0022	-0.0022	-0.0295		
503.150	503.150	1.38860 00	1.38730 00	C-C013	0.0091	0.0091	0.0862		
513.150	513.150	1.45540 00	1.45810 00	C-C013	0.0914	0.0914	0.0834		
523.150	523.150	1.52760 00	1.52510 00	C-C025	0.1613	0.1613	0.1540		
533.150	533.150	1.58600 00	1.58870 00	C-C027	-0.1714	-0.1714	-0.1599		
543.150	543.150	1.65420 00	1.64900 00	C-C052	0.3148	0.3148	0.3064		
553.150	553.150	1.71310 00	1.70620 00	C-C070	0.4076	0.4076	0.3879		
563.150	563.150	1.76820 00	1.76020 00	C-C080	0.4501	0.4501	0.4422		
573.150	573.150	1.82270 00	1.81150 00	C-C112	0.6152	0.6152	0.5902		
583.150	583.150	1.87380 00	1.86000 00	C-C138	0.7385	0.7385	0.7283		
593.150	593.150	1.92270 00	1.90580 00	C-C165	0.8815	0.8815	0.8921		
603.150	603.150	1.96540 00	1.94890 00	C-C205	1.0403	1.0403	1.0243		
613.150	613.150	2.01490 00	1.98950 00	C-C254	1.2617	1.2617	1.2711		
623.150	623.150	2.05760 00	2.02740 00	C-C296	1.4376	1.4376	1.4785		

-2C (L)	-1.300	8.6459C29D C1	-1.7282928D-02	0.0	-5.7691655D 04	-1.0971925D 02	5.2422476D-03
		2.3565007D C1					
		-1.0695478D C3					
REACTION CONSTANTS		'A'/'G'	'B'	'C'	'D'	'E'	'F'
		-2.1834049D C1	2.0565354D-02	-5.3338325D 04	1.2531818D 04	1.5259884D 02	-5.3572991D-03
		1.1560068D C3					

13/31/73

PROBLEM 1, THE SYSTEM H₂O AND THE SELF-IONIZATION OF WATER.

P20(L) = H₂O(G), LOG K. MAAS, 1970



PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

10/31/73

TEMPERATURE		HT2-HT1		ERROR	
T(2)	T(1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT
OSBECNE, STIMSON, AND GINNINGS, 1939					
276.150	273.160	9.0537C 01	5.0279D 01	0.2590	0.2950
283.150	273.160	1.8079C 02	1.8062D 02	0.1665	0.0921
289.150	273.160	2.7087D 02	2.7085D 02	0.0190	0.0370
293.150	273.160	3.6085D 02	3.6130D 02	-0.1444	-0.0400
298.150	273.160	4.5076D 02	4.5136D 02	-0.1444	-0.0400
303.150	273.160	5.4063D 02	5.4106D 02	-0.4297	-0.0795
308.150	273.160	6.3050D 02	6.3101D 02	-0.5071	-0.0804
313.150	273.160	7.2037C 02	7.2092C 02	-0.2475	-0.0760
318.150	273.160	8.1024D 02	8.1081D 02	-0.2645	-0.0697
323.150	273.160	9.0015D 02	9.0069D 02	-0.3370	-0.0557
328.150	273.160	9.9007D 02	9.9057D 02	-0.4561	-0.0501
333.150	273.160	1.1801D 03	1.1805D 03	-0.4290	-0.0389
338.150	273.160	1.1701D 03	1.1704D 03	-0.3229	-0.0276
343.150	273.160	1.2602D 03	1.2640D 03	-0.2191	-0.0174
348.150	273.160	1.3503D 03	1.3504D 03	-0.1047	-0.0078
353.150	273.160	1.4406D 03	1.4406D 03	0.0058	0.0004
358.150	273.160	1.5305D 03	1.5308D 03	0.1161	0.0076
363.150	273.160	1.6213D 03	1.6211D 03	0.2116	0.0130
368.150	273.160	1.7118D 03	1.7115D 03	0.3136	0.0183
373.150	273.160	1.8025D 03	1.8021D 03	0.4074	0.0226
378.150	273.160	1.8932D 03	1.8928D 03	0.4059	0.0214
383.150	273.160	1.9841D 03	1.9837D 03	0.4562	0.0230
388.150	273.160	2.0753D 03	2.0748D 03	0.5070	0.0244
393.150	273.160	2.1666D 03	2.1660C 03	0.5427	0.0251
398.150	273.160	2.2580D 03	2.2575D 03	0.5477	0.0243
403.150	273.160	2.3492D 03	2.3492D 03	0.5060	0.0215
408.150	273.160	2.4417D 03	2.4411D 03	0.5814	0.0238
413.150	273.160	2.5335D 03	2.5333C 03	0.5773	0.0228
418.150	273.160	2.6263D 03	2.6258D 03	0.4766	0.0181
423.150	273.160	2.7190D 03	2.7186D 03	0.4422	0.0163
428.150	273.160	2.8119D 03	2.8116D 03	0.2760	0.0098
433.150	273.160	2.9052D 03	2.9053D 03	0.1497	0.0048
438.150	273.160	2.9980D 03	2.9988D 03	0.1945	0.0065
443.150	273.160	3.0920C 03	3.0929D 03	0.0905	0.0020
448.150	273.160	3.1873D 03	3.1875D 03	-0.1027	-0.0332
453.150	273.160	3.2822D 03	3.2824D 03	-0.1364	-0.0421
458.150	273.160	3.3775D 03	3.3777D 03	-0.2421	-0.0722
463.150	273.160	3.4731D 03	3.4736D 03	-0.4462	-0.0128
468.150	273.160	3.5694D 03	3.5690D 03	-0.4105	-0.0115
473.150	273.160	3.6660D 03	3.6667C 03	-0.7028	-0.0192
478.150	273.160	3.7636D 03	3.7640D 03	-0.6307	-0.0168
483.150	273.160	3.8612D 03	3.8619D 03	-0.7647	-0.0158
488.150	273.160	3.9597D 03	3.9604D 03	-0.7771	-0.0146
493.150	273.160	4.0587D 03	4.0586D 03	-0.8830	-0.0218
498.150	273.160	4.1586D 03	4.1584D 03	-0.7654	-0.0183
503.150	273.160	4.2591D 03	4.2599D 03	-0.8112	-0.0190
508.150	273.160	4.3605D 03	4.3612D 03	-0.7209	-0.0165
513.150	273.160	4.4628D 03	4.4633D 03	-0.5401	-0.0121
518.150	273.160	4.5659D 03	4.5663D 03	-0.3246	-0.0071
523.150	273.160	4.6700D 03	4.6701D 03	-0.1369	-0.0029
528.150	273.160	4.7752D 03	4.7750D 03	0.1333	0.0028
533.150	273.160				
538.150	273.160				
543.150	273.160				
548.150	273.160				
553.150	273.160				
558.150	273.160				
563.150	273.160				
568.150	273.160				
573.150	273.160				
578.150	273.160				
583.150	273.160				
588.150	273.160				
593.150	273.160				
598.150	273.160				
603.150	273.160				
608.150	273.160				
613.150	273.160				
618.150	273.160				
623.150	273.160				
628.150	273.160				
633.150	273.160				
638.150	273.160				
643.150	273.160				
648.150	273.160				
653.150	273.160				
658.150	273.160				
663.150	273.160				
668.150	273.160				
673.150	273.160				
678.150	273.160				
683.150	273.160				
688.150	273.160				
693.150	273.160				
698.150	273.160				
703.150	273.160				
708.150	273.160				
713.150	273.160				
718.150	273.160				
723.150	273.160				
728.150	273.160				
733.150	273.160				
738.150	273.160				
743.150	273.160				
748.150	273.160				
753.150	273.160				
758.150	273.160				
763.150	273.160				
768.150	273.160				
773.150	273.160				
778.150	273.160				
783.150	273.160				
788.150	273.160				
793.150	273.160				
798.150	273.160				
803.150	273.160				
808.150	273.160				
813.150	273.160				
818.150	273.160				
823.150	273.160				
828.150	273.160				
833.150	273.160				
838.150	273.160				
843.150	273.160				
848.150	273.160				
853.150	273.160				
858.150	273.160				
863.150	273.160				
868.150	273.160				
873.150	273.160				
878.150	273.160				
883.150	273.160				
888.150	273.160				
893.150	273.160				
898.150	273.160				
903.150	273.160				
908.150	273.160				
913.150	273.160				
918.150	273.160				
923.150	273.160				
928.150	273.160				
933.150	273.160				
938.150	273.160				
943.150	273.160				
948.150	273.160				
953.150	273.160				
958.150	273.160				
963.150	273.160				
968.150	273.160				
973.150	273.160				
978.150	273.160				
983.150	273.160				
988.150	273.160				
993.150	273.160				
998.150	273.160				

532.150	273.160	4.88140 03	4.88100 03	0.4075	0.4083	0.1669
538.150	273.160	4.98820 03	4.98810 03	0.7767	0.7767	0.3114
543.150	273.160	5.09550 03	5.09550 03	0.5559	0.5559	0.3766
548.150	273.160	5.20170 03	5.20630 03	1.2820	0.0265	0.5308
553.150	273.160	5.31530 03	5.31760 03	1.7308	0.0325	0.6508
558.150	273.160	5.43260 03	5.43360 03	2.0339	0.3374	0.7498
563.150	273.160	5.54780 03	5.54540 03	2.4748	0.3446	0.8522
568.150	273.160	5.66490 03	5.66220 03	2.6680	0.0471	0.9420
573.150	273.160	5.78410 03	5.78130 03	2.7335	0.0473	0.9452
578.150	273.160	5.90580 03	5.90310 03	2.7492	0.0466	0.5310
583.150	273.160	6.03020 03	6.02770 03	2.5615	0.3425	0.8496
588.150	273.160	6.15770 03	6.15560 03	2.1350	0.0347	0.6934
593.150	273.160	6.28660 03	6.28130 03	1.2572	0.0216	0.4217
598.150	273.160	6.42350 03	6.42330 03	0.2017	0.0331	0.0628
603.150	273.160	6.56320 03	6.56430 03	-1.2955	-0.0197	-0.3948
608.150	273.160	6.70620 03	6.71120 03	-3.0641	-0.0457	-0.5136
613.150	273.160	6.85520 03	6.86500 03	-5.1580	-0.0839	-1.6789
618.150	273.160	7.01630 03	7.02690 03	-8.6423	-0.1231	-2.4628
623.150	273.160	7.18770 03	7.19640 03	-10.7369	-0.1494	-2.5876
628.150	273.160	7.37120 03	7.38150 03	-10.3599	-0.1405	-2.8109
633.150	273.160	7.57410 03	7.57860 03	-2.5358	-0.0335	-0.6654
638.150	273.160	7.81700 03	7.79270 03	24.2779	0.3106	6.2116

THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----

THE STANDARD DEVIATIONS ABOUT THE MEAN ARE -----

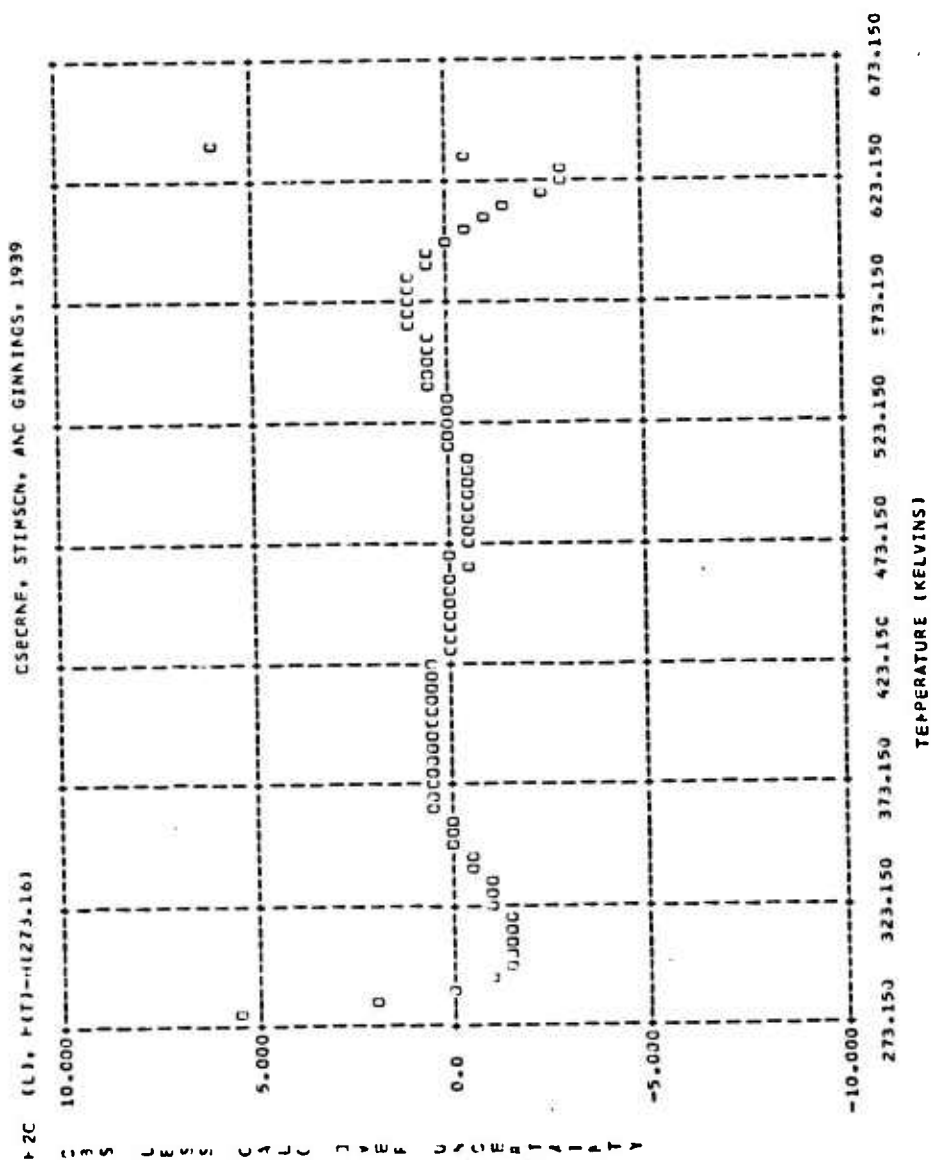
THE NUMBER OF OBSERVATIONS IS 73

10/31/73-----

PHASE	COEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
42C (L)	1.000	2.35650070 C1	-1.72825280-02	0.0	-5.76916550 04	-1.09719290 02	5.24225760-05
		-1.06954780 C3					
42C (L)	-1.000	2.35650070 C1	-1.72825280-02	0.0	-5.76916550 04	-1.09719290 02	5.24225760-05
		-1.06954780 C3					

10/31/73

PROBLEM 1, THE SYSTEM H₂O AND THE SELF-IGNITION OF WATER.



10/31/73

PROBLEM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

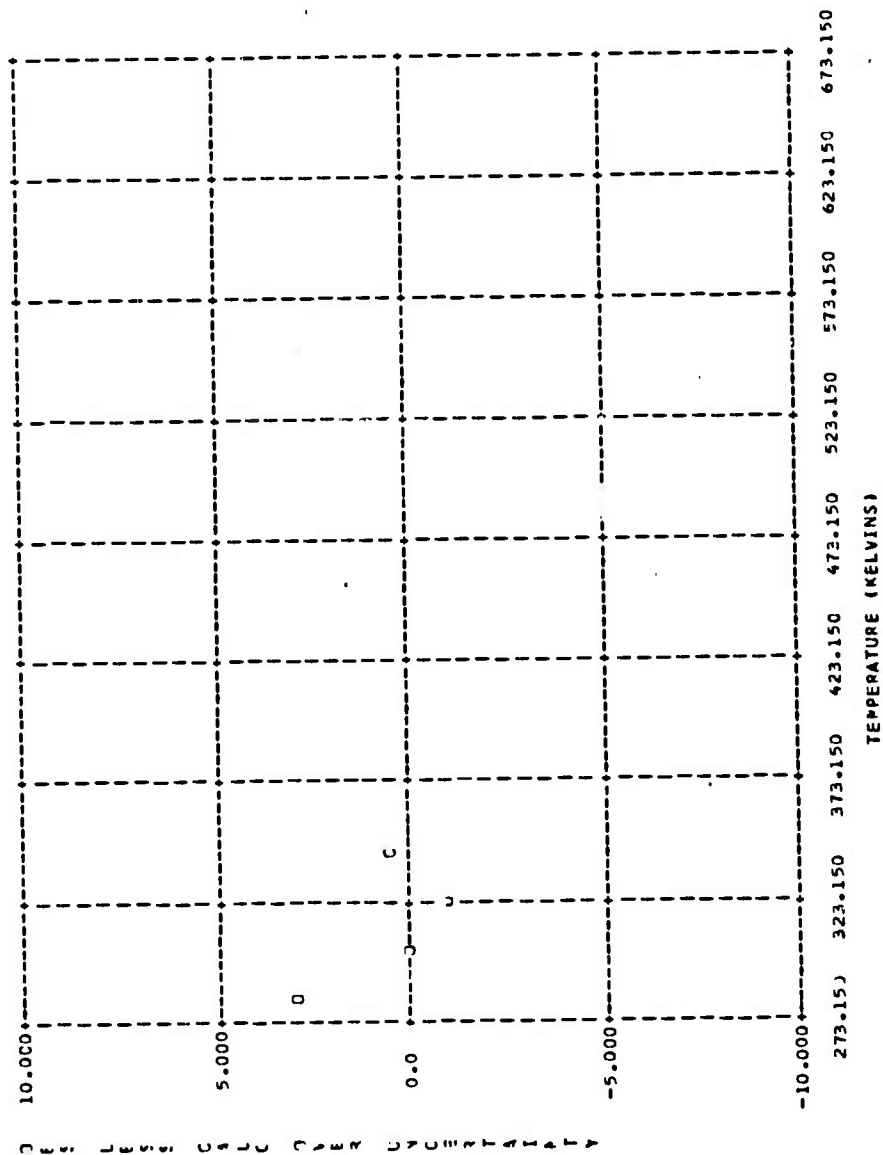
TEMPERATURE		HEAT CAP		ERROR	
T(2)	T(1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT
H+ + OH- = H2O(l), DELTA CP, REACTION, ACKERMANN, 1958.					
283.150	0.0	6.92000 D1	6.05940 D1	8.6057	12.4360
303.150	0.0	5.01000 D1	5.00840 D1	0.0164	0.0055
323.150	0.0	4.18000 D1	4.40630 D1	-2.2627	-5.4131
343.150	0.0	4.23000 D1	4.15270 D1	0.7733	1.8282
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----					
				1.7832	2.2210
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE -----					
				4.0944	6.4724
THE NUMBER OF OBSERVATIONS IS 4					
				0.5944	1.3648

10/31/73

PHASE	CHIEF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
H2O (L)	1.000	2.35650070 C1	-1.72829280-02	0.0	-5.76916550 D4	-1.09715290 D2	5.24229760-05
H+	-1.000	0.0	0.0	0.0	0.0	0.0	0.0
OH-	-1.000	3.53176540 C2	-3.56709830-01	-1.55304120 D7	-1.64048200 D5	-1.88952970 D3	0.0
REACTION CONSTANTS							
		'A'/'G'	'B'/'G(ION)'	'C'	'D'	'E'	'F'
		-3.25611530 C2	3.39426900-01	0.0	1.06356540 D5	1.77981040 D3	5.24229760-05
		-1.06954780 C3	1.55304120 D7				

PROBLEM 1. THE SYSTEM H₂O AND THE SELF-IONIZATION OF WATER.

$H_2O + OH^- \rightleftharpoons H_2O(L)$, DELTA CP, REACTION. ACKERMANN, 1958.



10/1/73

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

TEMPERATURE		ENTHALPY		ERROR	
T(2)	T(1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT ORS-CALC/SIGMO
298.150	0.0	1.33650 04	1.33650 04	-0.2473	-0.0019
323.150	0.0	1.21700 04	1.21750 04	-6.6628	-0.0383
347.550	0.0	1.11540 04	1.11420 04	12.6304	0.1132
373.550	0.0	1.00550 04	1.00570 04	-1.6454	-0.0164
398.450	0.0	8.92650 03	8.74200 03	-15.1334	-0.1695
417.750	0.0	7.99470 03	7.98300 03	11.7039	0.1464
					2.4484

P2C = CH + H₂O, HEAT OF IONIZATION OLOFSSON AND OLOFSSON, 1973.

THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----

THE STANDARD DEVIATIONS ABOUT THE MEAN ARE -----

THE NUMBER OF OBSERVATIONS IS 6

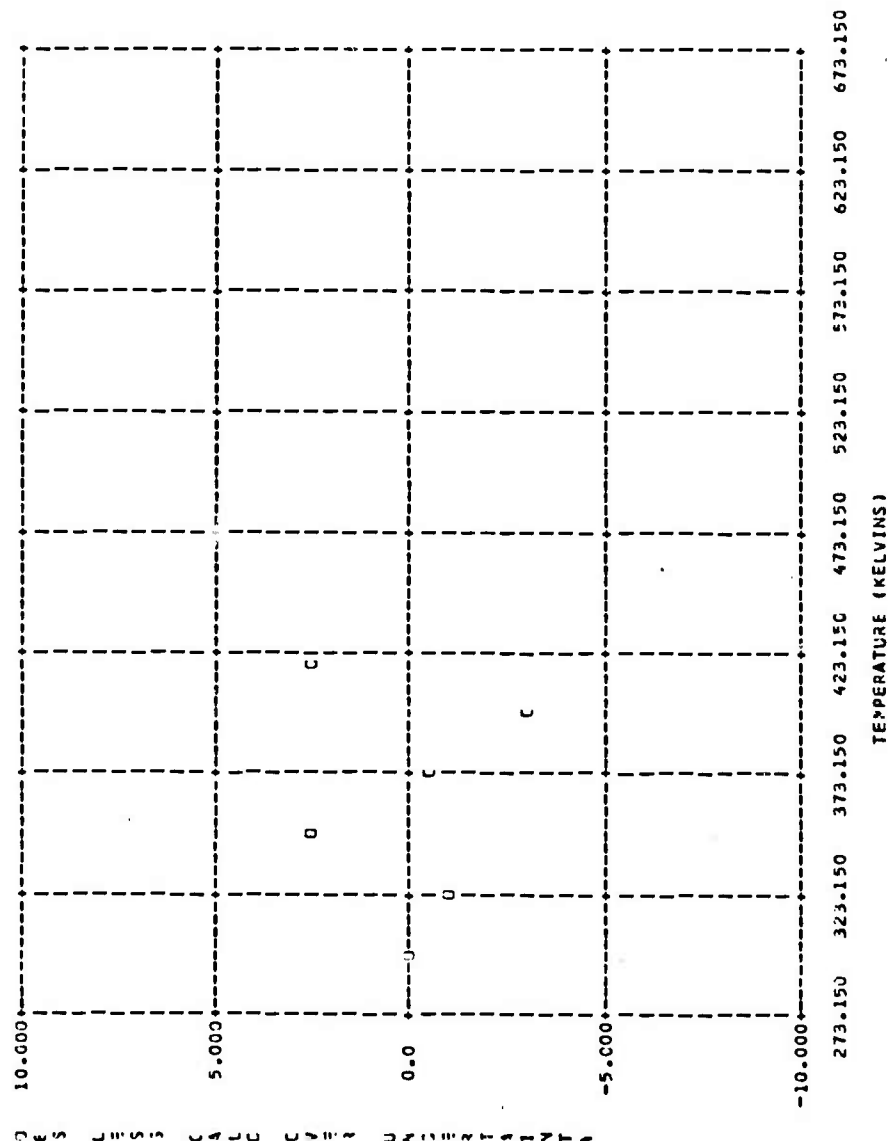
0.4402 0.0056 0.0921
9.5646 0.1037 2.0009

10/31/73-----									
PHASE	SELF	'A'/'G'	'B'	'C'	'D'	'E'	'F'	'G'	'H'
P2C (L)	-1.000	2.35650070 C1 -1.06954780 C3	-1.72829280-02	0.0	-5.76916550 04	-1.09719290 02	-1.09719290 02	5.76916550 04	5.76916550 04
M+	1.000	0.0 0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
M-	1.000	3.53176540 C2 0.0	-3.56705830-01	-1.55304120 07	-1.64048200 05	-1.88952970 03	-1.88952970 03	0.0	0.0
REACTION CONSTANTS		'A'/'G'	'B'/'G'110N1'	'C'	'D'	'E'	'F'	'G'	'H'
		3.29611530 C2 1.06954780 C3	-3.39426500-01 -1.55304120 07	0.0	-1.06356540 05	-1.77981040 03	-1.77981040 03	-5.24229160 03	-5.24229160 03

10/31/73

PROBLEM 1, THE SYSTEM H₂O AND THE SELF-IONIZATION OF WATER.

P-20 = CH- + H⁺, HEAT OF IONIZATION CLOFFSON AND CLOFFSON, 1973.



10/31/73

PROBLEM 1. THE SYSTEM H2C AND THE SELF-IONIZATION OF WATER.

LOG K _w	TEMPERATURE		LOG K	DIFFERENCE		PERCENT	OPS-CALC/SIGMO
	T(1)	T(2)	OBSERVED	CALCULATED	RIGNOLD, RPLWES, AND HEARN, 1971.		
324.150	0.0	0.0	-1.32410 01	-1.32540 01	0.0150	0.1129	0.7120
334.050	0.0	0.0	-1.25520 01	-1.30180 01	0.0259	0.1993	1.2331
343.050	0.0	0.0	-1.28020 01	-1.28080 01	0.0059	0.0462	0.4551
353.150	0.0	0.0	-1.26420 01	-1.26140 01	-0.0280	-0.2219	-2.8047
363.050	0.0	0.0	-1.26520 01	-1.24370 01	-0.0532	-0.4261	-1.9006
372.450	0.0	0.0	-1.22340 01	-1.22800 01	0.0459	0.3754	1.1778
381.750	0.0	0.0	-1.20750 01	-1.21390 01	0.0661	0.5312	2.5455
391.150	0.0	0.0	-1.19660 01	-1.20380 01	0.0216	0.1803	1.5440
400.450	0.0	0.0	-1.18700 01	-1.18900 01	0.0205	0.1724	1.4614
409.850	0.0	0.0	-1.17670 01	-1.17820 01	0.0152	0.1296	0.7625
419.150	0.0	0.0	-1.17210 01	-1.16860 01	-0.0348	-0.2970	-1.4502
428.550	0.0	0.0	-1.16080 01	-1.15980 01	-0.0092	-0.0792	-0.5410
437.850	0.0	0.0	-1.15480 01	-1.15210 01	-0.0266	-0.2304	-1.7737
447.350	0.0	0.0	-1.14730 01	-1.14510 01	-0.0215	-0.1872	-2.6846
456.750	0.0	0.0	-1.13530 01	-1.13910 01	-0.0018	-0.0160	-0.2273
466.150	0.0	0.0	-1.13230 01	-1.13390 01	0.0067	0.0589	0.4768
475.650	0.0	0.0	-1.12750 01	-1.12950 01	0.0162	0.1437	2.0258
485.250	0.0	0.0	-1.12590 01	-1.12590 01	0.0003	0.0024	0.0343
494.850	0.0	0.0	-1.12380 01	-1.12310 01	0.0023	0.0200	0.2814
504.550	0.0	0.0	-1.12160 01	-1.12100 01	-0.0057	-0.0504	-0.7065
514.350	1.0	1.0	-1.12020 01	-1.11970 01	-0.0052	-0.0473	-0.6618
524.150	0.0	0.0	-1.11560 01	-1.11910 01	-0.0041	-0.0367	-0.4561
534.150	0.0	0.0	-1.12040 01	-1.11940 01	-0.0099	-0.0887	-1.1036
544.150	0.0	0.0	-1.12200 01	-1.12040 01	-0.0158	-0.1404	-0.9265

THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----

11% STANDARD DEVIATIONS ABOUT THE MEAN ARE -----

THE NUMBER OF OBSERVATIONS IS 24

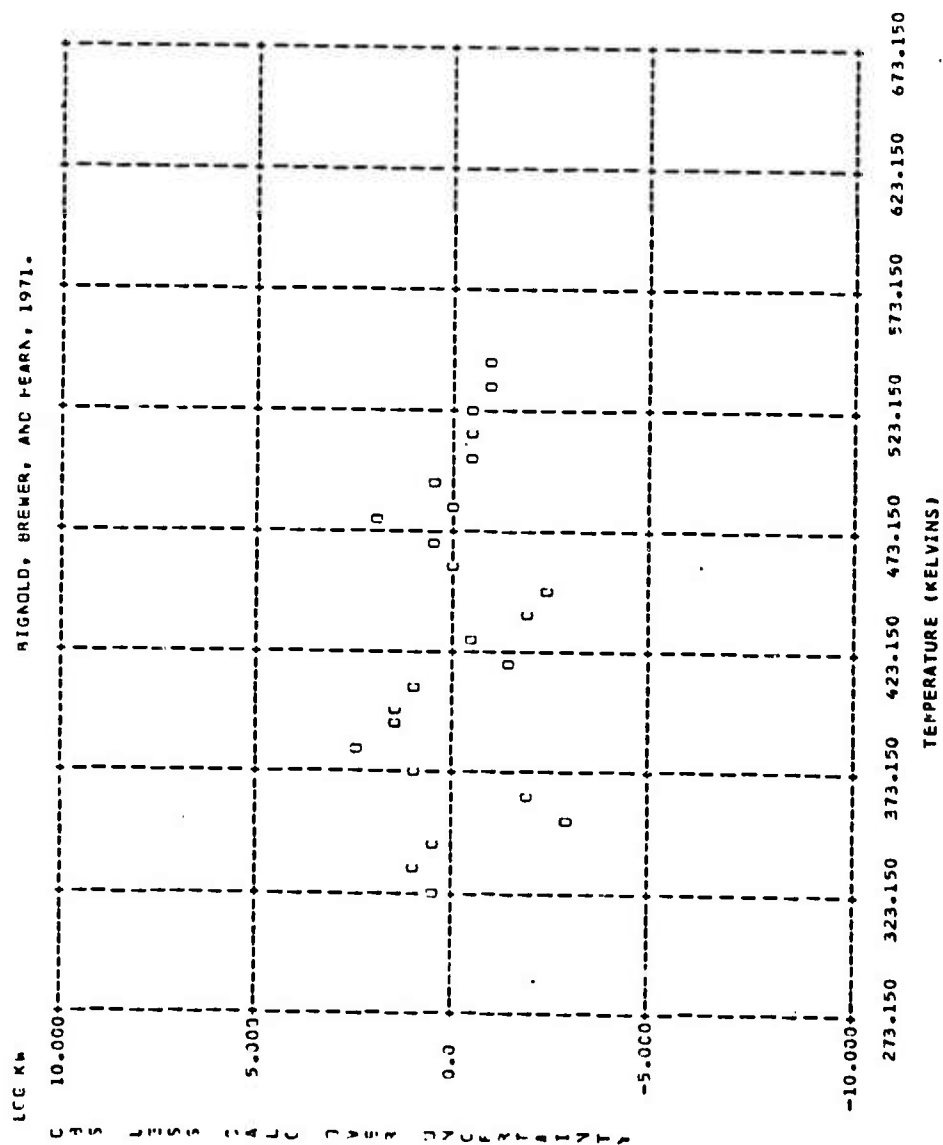
10/31/73		LOG K		DIFFERENCE		PERCENT		OPS-CALC/SIGMO	
PHASE	C/JEF	A*/G*	B*	C*	D*	E*	F*	G*	H*
P2C (L)	-1.000	2.25650070 C1 -1.06954780 C3	-1.72829280-02	0.0	-5.76916550 04	-1.09719290 02	5.24229760-05		
P+	1.000	0.0 0.0	0.0	0.0	0.0	0.0	0.0		
CH-	1.000	3.53176540 C2 0.0	-3.56709230-01	-1.55304120 07	-1.64048200 05	-1.88952970 03	0.0		

REACTION CCASSTANTS	3-2961153D C2	-3-3942690D-01	-1.0635654D 05	-1.7798104D 03	-5.2422976D-05
	1.0695478D C3	-1.5530412D C7			

0-0

10/11/73

PROBLEM 1: THE SYSTEM H₂O AND THE SELF-IGNITION OF WATER.



10/31/73

PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

TEMPERATURE		LOG K		FRRCR	
T (2)	T (1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT
-42C = CH - 4 H+, LOG KW.					
273.150	0.0	-1.49410 01	-1.49510 01	0.0102	0.0680
323.150	0.0	-1.32720 01	-1.32810 01	0.0092	0.0701
373.150	0.0	-1.22640 01	-1.22690 01	0.0051	0.0418
423.150	0.0	-1.16420 01	-1.16480 01	0.0055	0.0475
473.150	0.0	-1.13020 01	-1.13060 01	0.0040	0.0355
523.150	0.0	-1.11560 01	-1.11520 01	-0.0043	-0.0385
573.150	0.0	-1.13010 01	-1.12750 01	-0.0255	-0.2257
SWEETON, MESMER & BAES, PERS CPM, 1973.					
				0.0680	1.1282
				0.0701	1.5512
				0.0418	0.5698
				0.0475	0.4610
				0.0355	0.3342
				-0.0385	-0.2875
				-0.2257	-0.5669

THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----

THE STANDARD DEVIATIONS ABOUT THE MEAN ARE -----

THE NUMBER OF OBSERVATIONS IS 7

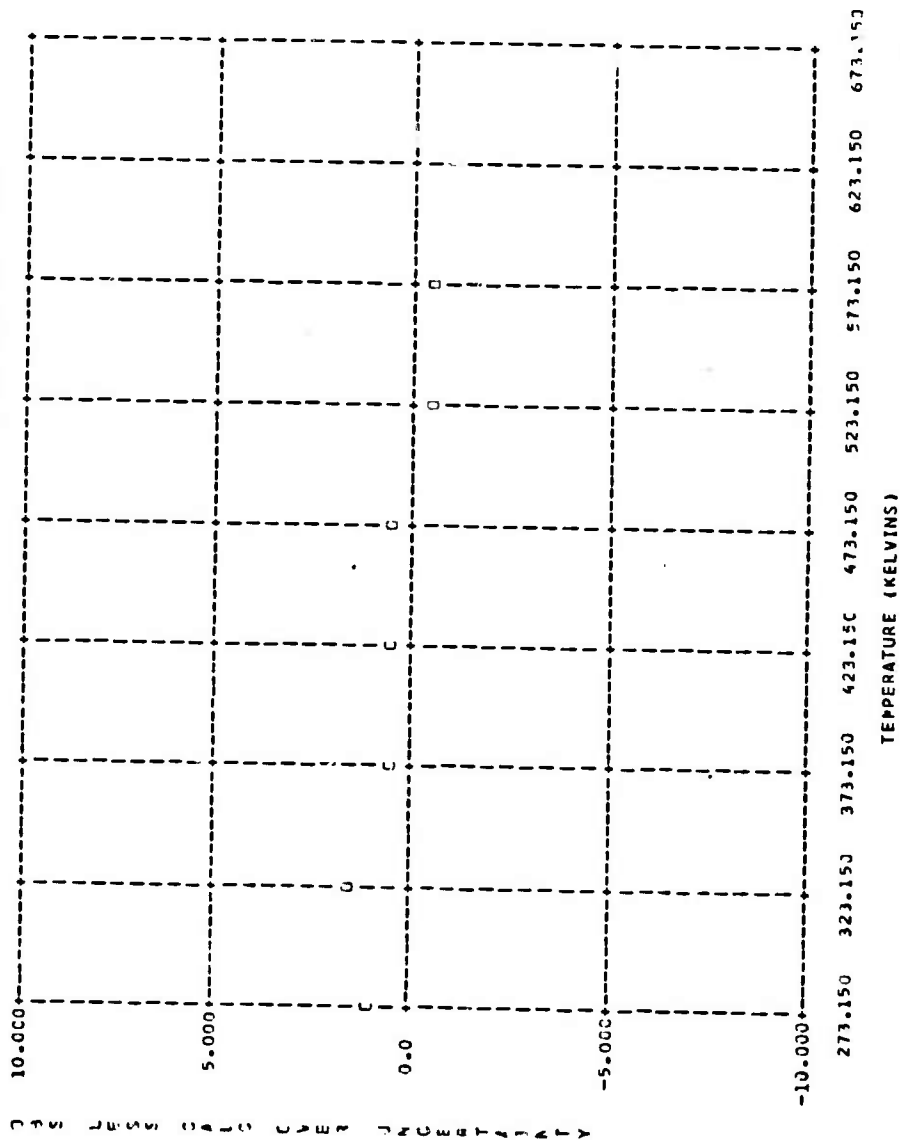
0.0006 -0.0002 0.4557
0.0115 0.0980 0.6843

IC/31/73-----									
PHASE	C DEF	'A'/'G'	'B'	'C'	'C'	'C'	'E'	'F'	'F'
P-20 (L)	-1.000	2.35650370 C1 -1.06954780 C3	-1.72829280-02	0.0	-5.76916550 J4	-1.09719290 02	5.2422970 J-05		
4+	1.000	0.0 0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0P-	1.000	3.53176540 C2 0.0	-3.56709830-01	-1.55304120 07	-1.64048200 05	-1.88952970 J3	C-C		
REFRACTION CONSTANTS									
		'A'/'G'	'B'/'G(ION)'	'C'	'D'	'E'	'F'		
		3.29611530 C2 1.06954780 C3	-3.39426500-01 -1.55304120 07	0.0	-1.06356540 05	-1.77981040 J3	-5.2422970 J-05		

PROBLEM 1, THE SYSTEM H₂O AND THE SELF-IONIZATION OF WATER.

10/31/73

H₂O = CH₂ + H₂, LOG KW. SWEETON, PESMER & BAES, PERE CCMM, 1973.



THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73
 PROBLEM 1. THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

WTC (G)	HEAT CAP	ENTROPY	ENTHALPY	GIBBS EN	LCG K	CELL EMF	P12-WT1
273.15	7.985	44.404	-41389.	-53517.	42.8158	2.3207	-200.
298.15	8.423	45.105	-41188.	-54636.	40.6496	2.3652	C.
400.00	8.193	47.485	-40362.	-55357.	32.4212	2.5739	825.
500.00	6.409	49.335	-39533.	-64201.	28.0623	2.7840	1655.
600.00	8.667	50.891	-38680.	-65214.	25.2113	3.0314	2505.
700.00	8.952	52.248	-37799.	-74373.	23.2202	3.2251	3385.
800.00	9.250	53.463	-36885.	-75659.	21.7619	3.4543	4245.
900.00	9.554	54.570	-35949.	-85062.	20.6558	3.6886	5240.
1000.00	9.857	55.552	-34978.	-90571.	19.7942	3.9274	6210.
1100.00	10.154	56.546	-33978.	-96178.	19.1088	4.1706	7211.
1200.00	10.442	57.442	-32948.	-101878.	18.5545	4.4178	8241.
1300.00	10.718	58.288	-31890.	-107665.	18.1001	4.6687	9259.
1400.00	10.981	59.092	-30805.	-113534.	17.7234	4.9232	10384.
1500.00	11.229	59.859	-29694.	-115482.	17.4085	5.1811	11455.
1600.00	11.461	60.591	-28559.	-125505.	17.1431	5.4423	12629.
1700.00	11.676	61.292	-27402.	-131599.	16.9182	5.7066	13786.
1800.00	11.873	61.965	-26225.	-137762.	16.7266	5.9738	14564.
1900.00	12.052	62.612	-25028.	-143991.	16.5627	6.2439	16160.
2000.00	12.211	63.234	-23815.	-150284.	16.4222	6.5168	17374.

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73
PROGRAM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

P2C (L)	HEAT CAP	ENTRCPY	ENTHALPY	GIBBS EN	LOG K	CELL EMP	P12-P11
273.15	18.195	15.051	-52185.	-56296.	45.0422	2.4412	C.
298.15	18.006	16.631	-51734.	-56693.	41.5568	2.4584	0.
323.15	17.976	18.080	-51284.	-57127.	38.6354	2.4772	C.
348.15	18.016	19.420	-50835.	-57596.	36.1555	2.4975	C.
373.15	18.128	20.673	-50383.	-58097.	34.0268	2.5193	0.
398.15	18.316	21.854	-49928.	-58629.	32.1821	2.5423	C.
423.15	18.584	22.977	-49466.	-59189.	30.5702	2.5666	0.
448.15	18.944	24.054	-48998.	-59777.	29.1516	2.5921	C.
473.15	19.414	25.094	-48518.	-60392.	27.8951	2.6188	C.
498.15	20.033	26.109	-48026.	-61032.	26.7760	2.6465	C.
523.15	20.875	27.109	-47515.	-61697.	25.7744	2.6754	C.
548.15	22.102	28.110	-46979.	-62387.	24.8740	2.7053	0.
573.15	24.075	29.135	-46404.	-63103.	24.0619	2.7363	0.
598.15	27.682	30.231	-45762.	-63845.	23.3273	2.7685	C.
623.15	35.393	31.500	-44987.	-64616.	22.6618	2.8019	0.
	'A'	'B'	'C'	'D'	'E'	'F'	'G'
2.35650070 01	-1.72829280-02	0.0	-5.76916550 04	-1.09719290 02	5.24229760-05	-1.66554780 03	

THESE RESULTS WERE OBTAINED IN A PLA CN 10/31/73
 PROBLEM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

	HEAT CAP	ENTRCPY	ENTHALPY	GIBBS FN	LCG K	CELL EMF	PT2-PT1
273.15	0.0	0.0	0.	0.	0.0	0.0	0.
298.15	0.0	0.0	0.	0.	0.0	0.0	0.
323.15	0.0	0.0	0.	0.	0.0	0.0	0.
348.15	0.0	0.0	0.	0.	0.0	0.0	0.
373.15	0.0	0.0	0.	0.	0.0	0.0	0.
398.15	0.0	0.0	0.	0.	0.0	0.0	0.
423.15	0.0	0.0	0.	0.	0.0	0.0	0.
448.15	0.0	0.0	0.	0.	0.0	0.0	0.
473.15	0.0	0.0	0.	0.	0.0	0.0	0.
498.15	0.0	0.0	0.	0.	0.0	0.0	0.
523.15	0.0	0.0	0.	0.	0.0	0.0	0.
548.15	0.0	0.0	0.	0.	0.0	0.0	0.
573.15	0.0	0.0	0.	0.	0.0	0.0	0.
598.15	0.0	0.0	0.	0.	0.0	0.0	0.
623.15	0.0	0.0	0.	0.	0.0	0.0	0.
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
'A'	'B'	'C'	'C'	'C'	'E'	'F'	'G'

THESE RESULTS WERE OBTAINED IN A RUN ON 10/21/73
 PROBLEM 1, THE SYSTEM H2O AND THE SELF-IONIZATION OF WATER.

CH-

	HEAT CAP	ENTRCPY	ENTHALPY	GIBBS FN	LOG K	CELL EMF	*12-+11
273.15	-49.846	1.004	-37336.	-37410.	30.0920	1.6309	0.
298.15	-54.238	-2.624	-38369.	-37586.	27.5514	1.6299	0.
323.15	-26.087	-5.015	-39109.	-37485.	25.3541	1.6256	0.
348.15	-23.330	-6.829	-39718.	-37340.	23.4401	1.6192	C.
373.15	-24.572	-8.470	-40305.	-37145.	21.7576	1.6109	0.
398.15	-26.841	-10.186	-40971.	-36916.	20.2637	1.6008	0.
423.15	-35.442	-12.131	-41771.	-36638.	18.9227	1.5987	0.
448.15	-43.870	-14.397	-42759.	-36307.	17.7057	1.5744	0.
473.15	-53.750	-17.038	-43976.	-35515.	16.5851	1.5574	0.
498.15	-64.797	-20.083	-45456.	-35451.	15.5534	1.5373	C.
523.15	-76.794	-23.544	-47224.	-34907.	14.5827	1.5137	C.
548.15	-89.572	-27.422	-49302.	-34271.	13.6639	1.4861	0.
573.15	-102.997	-31.712	-51708.	-33533.	12.7864	1.4541	0.
598.15	-116.963	-36.403	-54456.	-32682.	11.9412	1.4172	C.
623.15	-131.385	-41.484	-57560.	-31709.	11.1209	1.3750	C.
'A'	'B'	'C'	'D'	'E'	'F'	'G'	
3.53176540 02	-3.56709230-01	-1.55304120 07	-1.64048200 05	-1.88952970 03	0.0	0.0	0.0

Problem 2. The System Ni-O and the thermodynamics of Bunsenite (NiO).

As a second example, consider the selected calorimetric data for the following phases for the System Ni-O:

Ni (A) $\frac{3}{2}$	$T < 631 \text{ K}$ (Curie pernt)
Ni (B) $\frac{3}{2}$	$T > 631 \text{ K}$
Bunsenite $\frac{3}{2}$	$T < 525 \text{ K}$ (Curie pernt)
NiO (B) $\frac{3}{2}$	$525 \text{ K} < T < 565 \text{ K}$ (Transition point)
NiO (C)	$T > 565 \text{ K}$
O ₂ (G)	ideal gas, all T

The constants for nickel and oxygen are derived from an earlier regression and not refined in this problem. Only refined are the constants for Bunsenite, NiO(B), and NiO(C).

The data are the results of studies by E.G. King and his associates and include:

1. C_p (Bunsenite) from low temperature calorimetry
2. S_{298} (Bunsenite) from third law evaluation of low temperature calorimetry.
3. $H(T) - H(298)$ of Bunsenite from drop calorimetry.
4. $H(T)$ of NiO(B) - $H(298)$ of Bunsenite from drop calorimetry.
5. $H(T)$ of NiO(C) - $H(298)$ of Bunsenite from drop calorimetry.
6. ΔH_f° of Bunsenite from combustion calorimetry.

The input and results for this problem are given below.

Listing of input deck. The next two pages contain a listing of the input deck. Deleted from the input are the constants for Ni(A), Ni(B), and O₂(G) which were in the format (7A8).

$\frac{3}{2}$ There is no first-order structural change at the Curie pernt. However, because C_p is discontinuous, the mathematical model requires separate algebraic expressions for the temperature regions above and below the Curie pernt. The Curie pernt (and also all similar phenomenon) are treated here as "first" order transitions with mathematically derived ΔH and ΔS of "inversion" to describe the local anomaly.

PROBLEM 2, THE SYSTEM NiO AND THE THERMODYNAMICS OF PUNSENITE.

1 3 0 0 1
6 0 0
NI (A)NI (B)UNSENITNIO (B)NIO (C)OZ (G)
1 0 0 0 0 1

6
RUSSENFITE, HEAT CAPACITY

1	10	1	1	0	0	0
RUNSENIT	1.0000	00				0.001000 00
206.130	00			8.13400	00	0.001000 00
216.190	00			8.45700	00	0.001000 00
225.850	00			8.76200	00	0.001000 00
236.070	00			9.05000	00	0.001000 00
245.630	00			9.30600	00	0.001000 00
256.290	00			9.59700	00	0.001000 00
266.150	00			9.84500	00	0.001000 00
276.010	00			10.08000	00	0.001000 00
286.430	00			10.32000	00	0.001000 00
295.940	00			10.55000	00	0.001000 00

KING, E. G., JACS 79, 1957.

BUNSENITE, ENTPEPE

BUNSENITE	1	1	2	1	1	1	0	0	
BUNSENITE	1.0000	00			9.0000	00			0.040000 00

KING & CHRISTENSEN, JACS, 1958.

298.15D 00 9.030500
BUNSENITE, RELATIVE HEAT CONTENT.

BUNSENITE	2	5	7	1	1	0			
BUNSENITE	-1.00	00	00				0	0	
BUNSNITE	1.00	00	00				0	0	
364.900	00					0.75	00	03	0.002000 00
433.000	00					1.58	00	03	0.002000 00
502.900	00					2.58	00	03	0.002000 00
513.200	00					2.74	00	03	0.002000 00
524.200	00					2.92	00	03	0.002000 00

KING AND CHRISTENSEN, JACS, 1958.

524.200 JJ
NICKEL OXIDE, RELATIVE HEAT CONTENT

NID (P) 1.0000 00
525.000 00 565.000 00

525.000 00 565.000 00
BUNSFNITNIO (B)NIO (C)

BUNSENITE	-1.0000	00	0	0	
535.500	00	3.08000	03		0.002000 00
544.600	00	3.20500	03		0.002000 00
554.200	00	3.33500	03		0.002000 00
556.200	00	3.34500	03		0.002000 00
		3.44500	03		0.002000 00

KING AND CHRISTENSEN, JACS, 1958.

NICKEL OXIDE, RELATIVE HEAT CONTENT.

2 14 7 1 1 0

NIO (C) 1.0000 00
535.000 00 565.000 00

525.000 00 565.000 00
BUNSENITNIO (R)NIO (C)

BUNSENITE	-1.0000 00	0	0
572.300 00	3.58500 03	0.002000 00	
672.300 00	4.86500 03	0.002000 00	
795.700 00	6.31500 03	0.002000 00	
873.300 00	7.44000 03	0.002000 00	
964.900 00	8.62000 03	0.002000 00	
1088.800 00	10.21000 03	0.002000 00	
1206.900 00	11.75000 03	0.002000 00	
1224.400 00	12.02000 03	0.002000 00	
1304.300 00	13.12000 03	0.002000 00	

81

Printed output. The following pages contain a complete printed output from the execution of PHAS20 using the **preceding** data deck. By setting IL to 0, the results of the intermediate refinements were deleted. Constant 18, corresponding to the "d" constant for bunsenite, is the least significant of the constants included in the regression. If ICY had been set equal to or greater than 1, this constant would have automatically been set to 0.0 and the regression rerun.

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73
 PROBLEM 2, THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

PHASES CONSIDERED IN THIS REGRESSION ARE AS FOLLOWS---

NI (A)	NI (B)	BUNSENIT	NIO (A)	NIO (C)
C2 (G)				

10/31/73

PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

THE FOLLOWING DATA SLTS HAVE BEEN READ IN TC STORAGE:

SET NUMBER REFERENCE

1 KING, E. G., JACS 79, 1957.

BUNSENITE, HEAT CAPACITY

THE NUMBER OF PHASES IS: 1
THE NUMBER OF OBSERVATIONS IS: 10
THE TYPE OF DATA IS: HEAT CAP

PHASE NAME COEFFICIENT REF. STATE INVERSIONS

BUNSENIT	INDEX	COEFFICIENT	REF. STATE	INVERSIONS
		1.000	AC	0
			TEMPERATURE	
			T2	
	1	206.130		
	2	216.150		
	3	225.850		
	4	236.070		
	5	246.630		
	6	256.250		
	7	266.150		
	8	276.010		
	9	286.430		
	10	296.540		
			T1	
			HEAT CAP	
			ERROR	
				8.134C00-03
				8.457C00-03
				8.762C00-03
				9.053C00-03
				9.306C00-03
				9.597C00-03
				9.845C00-03
				1.008C00-02
				1.032C00-02
				1.055C00-02

2 KING, E. G., JACS 79, 1951.

BUNSENITE, ENTROPY

THE NUMBER OF PHASES IS: 1
THE NUMBER OF OBSERVATIONS IS: 1
THE TYPE OF DATA IS: ENTROPY

PHASE NAME COEFFICIENT REF. STATE INVERSIONS

BUNSENIT	INDEX	COEFFICIENT	REF. STATE	INVERSIONS
		1.000	AD	0
			TEMPERATURE	
			T2	
	11	296.150		
			T1	
			ENTROPY	
			ERROR	
				4.000C00-02

3 KING & CHRISTENSEN, JACS, 1958.

BUNSENITE, RELATIVE HEAT CONTENT.

THE NUMBER OF PHASES IS: 2
THE NUMBER OF OBSERVATIONS IS: 5
THE TYPE OF DATA IS: HT2-HT1

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
BUNSENIT	-1.000	NO	0
PLASENIT	1.000	NO	0

INDEX	T2	TEMPERATURE	T1	HT2-HT1	ERRCR
12	364.900		298.150	7.500000 02	1.500000 00
13	432.000		298.150	1.500000 03	3.160000 00
14	502.900		298.150	2.585000 03	5.170000 00
15	512.200		298.150	2.740000 03	5.400000 00
16	524.200		298.150	2.925000 03	5.850000 00

4 NICKEL OXIDE, RELATIVE HEAT CONTENT KING AND CHRISTENSEN, JACS, 1958.

THE NUMBER OF PHASES IS: 2
THE NUMBER OF OBSERVATIONS IS: 5
THE TYPE OF DATA IS: HT2-HT1

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
NTC (B)	1.000	NO	1

INVERSIONS ARE AS FOLLOWS:

1. JJ	BUNSENIT	NIO (B)	525.000
PLASENIT	-1.000	NO	0

INDEX	T2	TEMPERATURE	T1	HT2-HT1	ERRCR
17	535.500		298.150	3.680000 03	6.160000 00
18	544.600		298.150	3.205000 03	6.410000 00
19	554.200		298.150	3.335000 03	6.670000 00
20	556.200		298.150	3.345000 03	6.680000 00
21	561.200		298.150	3.445000 03	6.950000 00

5 NICKEL OXIDE, RELATIVE HEAT CONTENT. KING AND CHRISTENSEN, JACS, 1958.

THE NUMBER OF PHASES IS: 2
THE NUMBER OF OBSERVATIONS IS: 14
THE TYPE OF DATA IS: HT2-HT1

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
NTC (C)	1.000	NO	2

INVERSIONS ARE AS FOLLOWS:

1.00 BUNSENIT = N10 (P) 525.000
 1.00 N10 (P) = N10 (C) 565.000
 BUNSENIT -1.000 NC

INDEX	TEMPERATURE T2	TEMPERATURE T1	HT2-HT1	ERROR
22	572.300	298.150	3.585000 J3	7.170000 00
23	672.300	298.150	4.865000 J3	9.730000 00
24	785.700	298.150	6.315000 J3	1.262000 01
25	873.300	298.150	7.440000 J3	1.488000 01
26	964.900	298.150	8.620000 J3	1.724000 01
27	1088.800	298.150	1.021000 04	2.042000 01
28	1206.500	298.150	1.175000 04	2.350000 01
29	1224.400	298.150	1.202000 04	2.454000 01
30	1304.300	298.150	1.312000 04	2.624000 01
31	1406.300	298.150	1.454000 04	2.909000 01
32	1500.500	298.150	1.584000 04	3.168000 01
33	1604.400	298.150	1.736000 04	3.472000 01
34	1706.800	298.150	1.889000 04	3.776000 01
35	1805.700	298.150	2.044000 04	4.080000 01

BOYLE, KING, AND CONWAY, 1954.

BUNSENITE, HEAT OF FORMATION.

THE NUMBER OF PHASES IS: 3
 THE NUMBER OF OBSERVATIONS IS: 1
 THE TYPE OF DATA IS: ENTHALPY

PHASE NAME	COEFFICIENT	REF. STATE	INVERSIONS
BUNSENIT	1.000	NC	C
N1 (A)	-1.000	YES	C
C2 (G)	-0.500	YES	C

INDEX	TEMPERATURE T2	TEMPERATURE T1	ENTHALPY	ERROR
36	258.150	-	-5.730000 04	1.000000 02

THE INDEX OF THE LAST ITEM OF THE ABOVE DATA SETS IN THE VECTORS X(1:1), Y(1:1), AND SIGMA(1:1)
IS AS FOLLOWS:

DATA SET	INDEX
1	10
2	11
3	16
4	21
5	35
6	36

PROBLEM 2, THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

NUMBER OF CYCLES IN THIS JCR IS 3

NUMBER OF PARAMETERS TO BE VARIED IS 13

NUMBER OF INDEPENDENT VARIABLES PER OBSERVATION IS 2

DERIVATIVES PROGRAMMED IN SUBROUTINE EAFW20.

WEIGHTS TO BE SUPPLIED BY USER

NUMBER OF PARAMETERS READ IS 42

NUMBER OF OBSERVATIONS READ IS 36

TOTAL CONSTANTS

I P(I) K(I)

NI (A) 0
1 1.37040 01 0
2 -1.29020-02 0
3 -2.16220 05 0
4 0.0 0
5 -6.57710 01 0
6 2.57730-05 0
7 0.0 0

NI (B) 0
8 -3.10550 00 0
9 6.81430-03 0
10 1.47630 06 0
11 0.0 0
12 2.66100 01 0
13 -4.13150-06 0
14 0.0 0

BUNSENITE
15 1.00000 01 1
16 1.00000-08 1
17 1.00000-08 1
18 1.00000-06 1
19 1.00000 01 1
20 1.00000-08 1
21 1.00000-08 1

NI-O (d) 1
22 1.00000 01 1
23 0.0 0
24 0.0 0
25 0.0 0
26 1.00000 01 1
27 0.0 0
28 0.0 0

NI-O (C) 1
29 1.00000 01 1
30 1.00000-08 1
31 1.00000-08 1

32	0.0	0
33	1.0000 01	1
34	C.C	0
35	0.0	0
	C2 (C1)	
36	1.34590 01	0
37	-5.97400-04	0
38	1.61500 05	0
39	0.0	0
40	-4.18760 01	0
41	2.50800-07	0
42	-1.35900 02	0

PROBLEM 2, THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.
 BUNSENITE, HEAT CAPACITY KING, E. G., JACS 79, 1957.
 BUNSENITE, ENTROPY KING, E. G., JACS 79, 1957.
 BUNSENITE, RELATIVE HEAT CONTENT. KING & CHRISTENSEN, JACS, 1958.
 NICKEL OXIDE, RELATIVE HEAT CONTENT KING AND CHRISTENSEN, JACS, 1958.
 NICKEL OXIDE, RELATIVE HEAT CONTENT. KING AND CHRISTENSEN, JACS, 1958.
 BUNSENITE, HEAT OF FORMATION. BOYLE, KING, AND CONWAY, 1954.
 AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 1
 $SUM((O-C)**2)$ IS 0.2790 C7
 $SCRIPT(SUM((O-C)**2)/(NO-NV))$ IS 0.3481D C2

FIGURE 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

PARAMETERS AFTER LEAST SQUARES CYCLE 1

NI	(A)	OLD	CHANGE	NEW	ERROR	PCT. CHANGE	PCT. ERROR
1	1.37336280150 01		1.37336280150 C1				
2	-1.29019559040-02		-1.29019559040-C2				
3	-2.16223388110 05		-2.16223388110 C5				
4	0.0		0.0				
5	-6.57710667810 01		-6.57710667810 C1				
6	2.97703356390-05		2.97703356390-C5				
7	C.C		0.0				
8	-3.10546549470 00		-3.10546549470 C0				
9	6.81466261710-03		6.81466261710-C3				
10	1.47555546490 06		1.47555546490 C6				
11	0.0		0.0				
12	2.66102409970 01		2.66102409970 C1				
13	-4.13166688060-06		-4.13166688060-C6				
14	0.0		0.0				
BUNSENITE							
15	1.00000000000 01		2.17306655320 02	2.273066855320 02	3.96676685180 01	9.55946466510 01	17.4742
16	1.00000000000-08		-1.625903596010-01	-1.625903596010-C1	2.00455407510-02	1.00000000000 02	18.439
17	1.00000000000-08		8.55305775430 05	8.55305775430 C5	1.77553136140 C5	1.00000000000 C2	20.790
18	1.00000000000-08		-9.81501095410 03	-9.81501095410 C3	7.56361012710 C3	1.00000000000 02	77.2654
19	1.00000000000 01		-1.50803827640 03	-1.49803827640 03	2.45668333030 02	1.00000000000 02	17.6609
20	1.00000000000-08		2.61904164890-04	2.60914164890-04	4.46301480320-C5	9.59961673220 C1	17.119
21	1.00000000000-08		-2.62571055690 C3	-2.62571055690 C3	4.78906814440 02	1.00000000000 02	18.291
22	1.00000000000 01		3.72494487270 00	1.37249448730 01	5.02328885720-C1	2.71399623620 01	3.6000
23	0.0		0.0				
24	0.0		0.0				
25	0.0		0.0				
26	1.00000000000 01		-7.9707635510 C1	-6.97078635510 01	2.17048561380 00	1.143455583830 02	4.5482
27	C.C		0.0				
28	C.C		0.0				
29	1.00000000000 01		-1.53143586860 C0	8.46856413140 00	6.85611377170-01	-1.80837724650 01	8.1456
30	1.00000000000-08		1.82396744000-03	1.82397744000-03	2.21965082230-04	9.99994517480 01	12.1693
31	1.00000000000-08		8.36545797290 05	8.36545797290 C5	2.01802482770 05	1.00000000000 02	24.1232
32	C.C		0.0				
33	1.00000000000 01		-6.71432741140 C1	-3.71432741140 01	4.42425279450 C0	1.26922774680 02	11.9113
34	C.C		0.0				
35	C.C		0.0				
36	1.34066510000 01		1.34066510000 C1				
37	-5.57401480000-04		-5.57401480000-C4				
38	1.61901710000 05		1.61901710000 C5				
39	C.C		0.0				
40	-4.18778890000 01		-4.18778890000 C1				
41	2.50867120000-07		2.50867120000-C7				
42	-1.35923630000 02		-1.35923630000 C2				

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 1

$\{L^*(W(C-C)^{**2})\}$ IS 0.5880 C2

$\text{SQRTF}(\text{SUM}(L^*(U-C)^{**2})/(\text{NC-NV}))$ IS 0.15590 C1

PROBLEM 2, THE SYSTEM Ni-O AND THE THERMODYNAMICS OF BUNSENITE.
 ELASENITE, HEAT CAPACITY KING, E. G., JACS 79, 1957.
 BUNSENITE, ENTROPY KING, E. G., JACS 79, 1957.
 ELASENITE, RELATIVE HEAT CONTENT. KING & CHRISTENSEN, JACS, 1958.
 NICKEL OXIDE, RELATIVE HEAT CONTENT KING AND CHRISTENSEN, JACS, 1958.
 NICKEL OXIDE, RELATIVE HEAT CONTENT. KING AND CHRISTENSEN, JACS, 1958.
 ELASENITE, HEAT OF FORMATION. BOYLE, KING, AND CONWAY, 1954.
 AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 2
 SLP(1*(O-C)**2) IS 0.5940 02
 SCRT(SUM(W*(U-C)**2)/(ND-NV)) IS 0.16070 01

PROCEDURE 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF RUNSENITE.
PARAMETERS AFTER LEAST SQUARES CYCLE 2

		OLD	CHANGE	NEW	ERROR	PCT. CHANGE	PCT. ERROR
NI (A)							
1	1.37036280450 01		1.37036280150 C1				
2	-1.29015559340-02		-1.29015559340-C2				
3	-2.16220388110 05		-2.16220388110 C5				
4	C.C		0.0				
5	-6.57710667810 01		-6.57710667810 C1				
6	2.5770356390-05		2.5770356390-C5				
7	C.C		0.0				
NI (P)							
8	-3.10566549470 00		-3.10566549470 C0				
9	6.8148261710-03		6.8148261710-C3				
10	1.4755558450 06		1.4755558450 C6				
11	C.C		0.0				
12	2.66105709470 01		2.66105709470 C1				
13	-4.1314688060-06		-4.1314688060-C6				
14	C.C		0.0				
RUNSENITE							
15	2.27036285720 02		2.27036285720 C2				
16	-1.62950597070-01		-1.62950597070-C1				
17	8.55335775430 05		8.55335775430 C5				
18	-9.81501070490 03		-9.81501070490 C3				
19	-1.4903327640 03		-1.4903327640 C3				
20	2.6091166490-04		2.6091166490-C4				
21	-2.62571355690 03		-2.62571355690 C3				
NI (P)							
22	1.37249448730 01		1.37249448730 C1				
23	C.C		0.0				
24	0.0		0.0				
25	0.0		0.0				
26	-6.57076635510 01		-6.57076635510 C1				
27	C.C		0.0				
28	C.C		0.0				
NI (C)							
29	8.46856413140 00		8.46856413140 C0				
30	1.82397744300-03		1.82397744300-C3				
31	8.36547797290 05		8.36547797290 C5				
32	0.0		0.0				
33	-3.71432741140 01		-3.71432741140 C1				
34	C.C		0.0				
35	C.C		0.0				
NI (G)							
36	1.34046510000 01		1.34046510000 C1				
37	-5.97401483000-04		-5.97401483000-C4				
38	1.61901710000 05		1.61901710000 C5				
39	C.C		0.0				
40	-4.18778850000 01		-4.18778850000 C1				
41	2.50885120000-07		2.50885120000-C7				
42	-1.35920000000 02		-1.35920000000 C2				

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 2

$\sqrt{1/(N(C-C)^2)}$ IS 0.594E 02

$\sqrt{C/(SUM(N(J-C)^2)/(N-NV))}$ IS 0.16070 01

PROBLEM 2, THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.
 BUNSENITE, HEAT CAPACITY KING, E. G., JACS 79, 1957.
 BUNSENITE, ENTROPY KING, E. G., JACS 79, 1957.
 BUNSENITE, RELATIVE HEAT CONTENT. KING & CHRISTENSEN, JACS, 1958.
 NICKEL OXIDE, RELATIVE HEAT CONTENT KING AND CHRISTENSEN, JACS, 1958.
 NICKEL OXIDE, RELATIVE HEAT CONTENT. KING AND CHRISTENSEN, JACS, 1958.
 BUNSENITE, HEAT OF FORMATION. BOYLE, KING, AND CONWAY, 1954.

APPROXIMATE FACTORS BASED ON PARAMETERS BEFORE CYCLE 3

$SL(1+(10-C)^{0.2})$ IS 0.5940 02
 $SCPT(SUM(W(10-C)^{0.2})/(10-NV))$ IS 0.16070 01

PROBLEM 2, THE SYSTEM Ni-C AND THE THERMODYNAMICS OF BUNSENITE.
PARAMETERS AFTER LEAST SQUARES CYCLE 3

		CHANGE		NEW		ERROR		PCT. CHANGE		PCT. ERROR	
		OLD									
NI (J)											
1	1.37036280150 J1		1.37036280150 C1								
2	-1.259318559040-02		-1.259318559040-02								
3	-2.16223388110 05		-2.16223388110 C5								
4	C.C		0.0								
5	-6.57710667810 J1		-6.57710667810 C1								
6	2.57703565590-05		2.57703565590-05								
7	0.0		0.0								
VI (E)											
8	-3.10546549470 00		-3.10546549470 C0								
9	6.8148261710-03		6.8148261710-03								
10	1.4755554490 06		1.4755554490 C6								
11	C.C		0.0								
12	2.6610245570 C1		2.6610245570 C1								
13	-4.13146688060-06		-4.13146688060-06								
14	C.C		0.0								
BUNSENITE											
15	2.27000000000 02		2.27000000000 C2								
16	-1.62554670330-14		-1.62554670330-14								
17	8.55305764210 05		8.55305764210 C5								
18	-9.81501070490-03		-9.81501070490-03								
19	-1.4980338800-10		-1.4980338800-10								
20	3.34015718920-17		3.34015718920-17								
21	-2.62571057200 03		-2.62571057200 C3								
VI (E)											
22	1.37249448870 C1		1.37249448870 C1								
23	0.0		0.0								
24	C.C		0.0								
25	C.C		0.0								
26	-6.57070036380 01		-6.57070036380 C1								
27	C.C		0.0								
28	C.C		0.0								
VI (C)											
29	8.46856410960 00		8.46856410960 C0								
30	1.82337744690-03		1.82337744690-03								
31	8.3656703350 05		8.3656703350 C5								
32	C.C		0.0								
33	-3.71432739740 J1		-3.71432739740 C1								
34	0.0		0.0								
35	C.C		0.0								
12 (C)											
36	1.34006510000 01		1.34006510000 C1								
37	-5.57431480000-04		-5.57431480000-04								
38	1.61901710000 05		1.61901710000 C5								
39	C.C		0.0								
40	-4.1877490000 J1		-4.1877490000 C1								
41	2.5088120000-07		2.5088120000-07								
42	-1.3597006000 02		-1.3597006000 C2								

ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLE 3

SLM(L*(C-C)**2) IS 0.594D C2

SCPTF(SUM(W*(C-C)**2)/(NO-NV)) IS 0.1607D 01

SUBROUTINE TEST INDICATES THAT JOB IS TO BE TERMINATED FOR REASON 1

PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF PUNSENITE.

CORRELATION MATRIX

1	0.10000 0.0 -0.99870 00 0.99490 00 -0.56270-08 -0.55650-08 -0.38020-03	0.59850 00 -0.10000 01 0.99450 00 -0.99970 00 -0.50590-08 -0.53060-03 0.56660-08
2	0.0 0.10000 01 -0.99860 00 -0.59460 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08
3	0.0 0.0 0.10000 01 0.99860 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08
4	0.0 0.0 0.0 0.10000 01 0.99860 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08
5	0.0 0.0 0.0 0.0 0.10000 01 0.99860 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08
6	0.0 0.0 0.0 0.0 0.0 0.10000 01 0.99860 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08
7	0.0 0.0 0.0 0.0 0.0 0.0 0.10000 01 0.99860 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08
8	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.10000 01 0.99860 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08
9	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.10000 01 0.99860 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08
10	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.10000 01 0.99860 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08
11	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.10000 01 0.99860 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08
12	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.10000 01 0.99860 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08
13	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.10000 01 0.99860 00 0.99710 00 0.50550-08 0.54240-03 -0.56660-08	0.59850 00 -0.99950 00 0.99880 00 0.99710 00 -0.50550-08 -0.53060-03 0.56660-08

PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

10/31/73

TEMPERATURE		HEAT CAP		ERROR		
T(2)	T(1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT	OBS-CALC/SIGMO
BUNSENITE, HEAT CAPACITY						
KING, E. G., JACS 79, 1957.						
206.130	0.0	8.134CD 00	8.144JD 00	-0.0100	-0.1234	-1.2241
216.150	0.0	8.451CD 00	8.4491D 00	0.0019	0.0930	0.9205
225.850	0.0	8.762CD 00	8.7431D 00	0.0189	0.2156	2.1559
236.070	0.0	9.030CD 00	9.0467D 00	-0.0167	-0.0365	-0.3654
245.620	0.0	9.306CD 00	9.319CD 00	-0.0130	-0.1402	-1.4018
254.250	0.0	9.571CD 00	9.6065D 00	-0.0355	-0.0994	-0.9945
264.150	0.0	9.845CD 00	9.8562D 00	-0.0112	-0.1142	-1.1419
276.010	0.0	1.005CD 01	1.0090D 01	-0.0035	-0.1041	-1.0410
286.430	0.0	1.022CD 01	1.0322D 01	-0.0102	-0.0222	-0.2216
295.940	0.0	1.055CD 01	1.0521D 01	0.0029	0.0278	0.2780

THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----

THE STANDARD DEVIATIONS ABOUT THE MEAN ARE -----

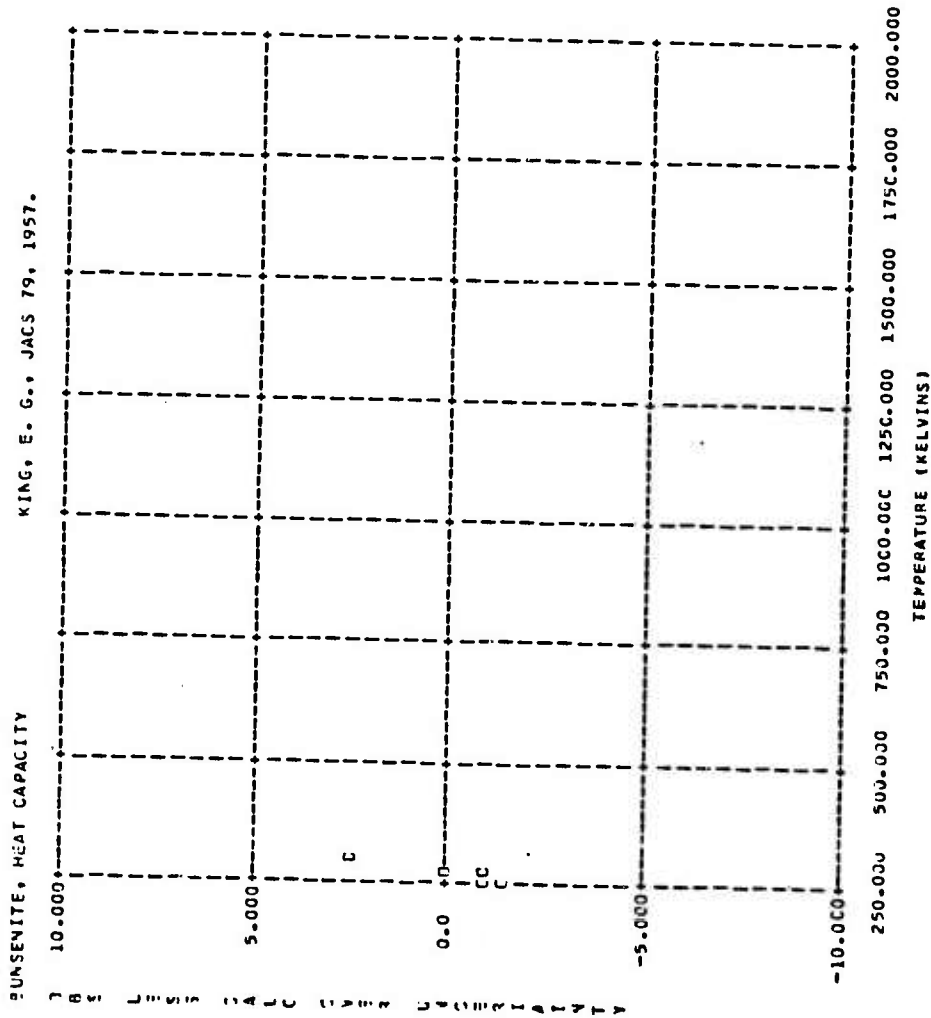
THE NUMBER OF OBSERVATIONS IS 10

10/31/73-----

PARAM	CDEF	TA/T/SG	'B'	'C'	'D'	'E'	'F'
BUNSENITE	1.000	2.270J6860 C2	-1.6299J60D-01	8.5530578C 05	-9.8150107D J3	-1.4980383D J3	2.6091417D-04
		-2.6257106D C3					

FIGURE 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF RUNSENITE.

10/31/73



10/31/73

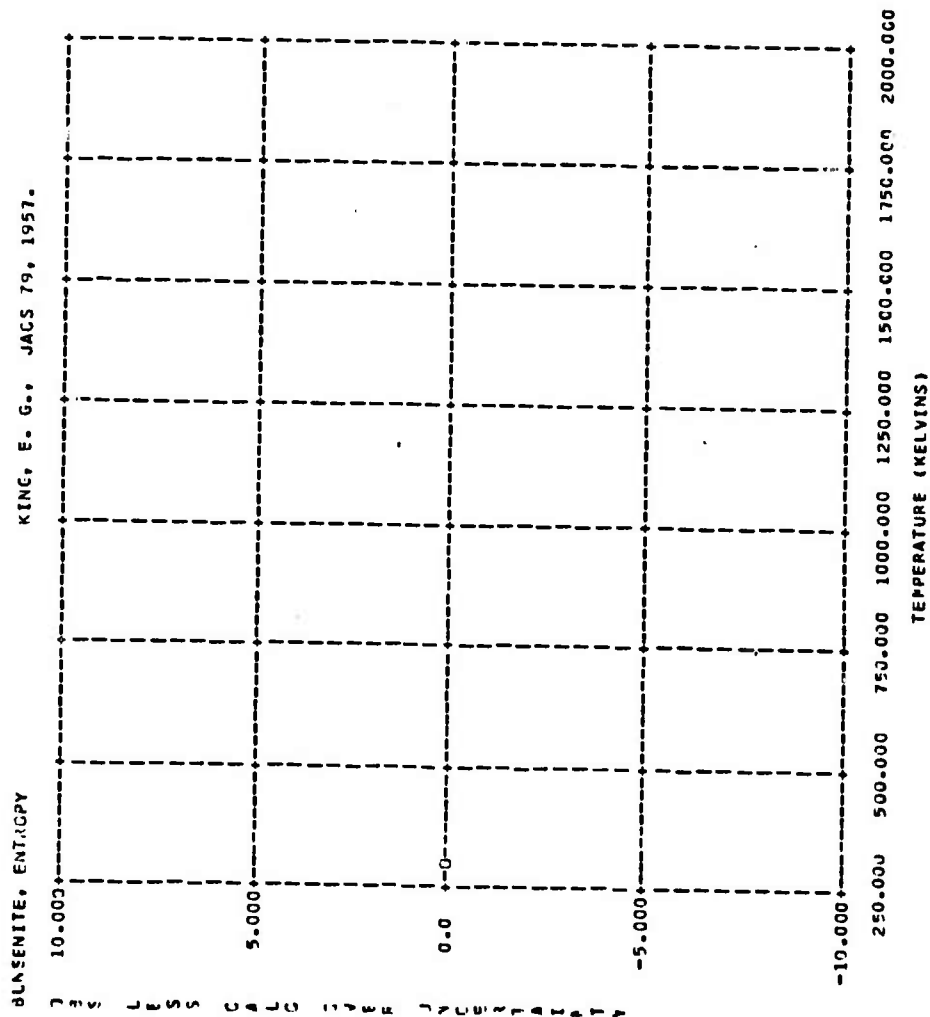
PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

TEMPERATURE		ENTROPY		ERROR	
T(2)	T(1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT
KING, E. G., JACS 79, 1957.					
298.150	0.0	9.08000 00	9.08000 00	0.0000	0.0000
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----					
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE -----					
THE NUMBER OF OBSERVATIONS IS 1					

10/31/73-----					
PHASE	COEF	'A'/'G'	'B'	'C'	'D'
BUNSENITE	1.000	2.27036860 C2	-1.62950600-01	8.55305780 05	-9.81501070 03
		-2.62571060 C3			-1.49803830 03
					2.60914170-04

10/31/73

FIGURE 2. THE SYSTEM Ni-O AND THE THERMODYNAMICS OF BUNSENITE.



THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----

THE STANCARD DEVIATIONS ABOUT THE MEAN ARE -----

THE NUMBER OF OBSERVATIONS IS 5

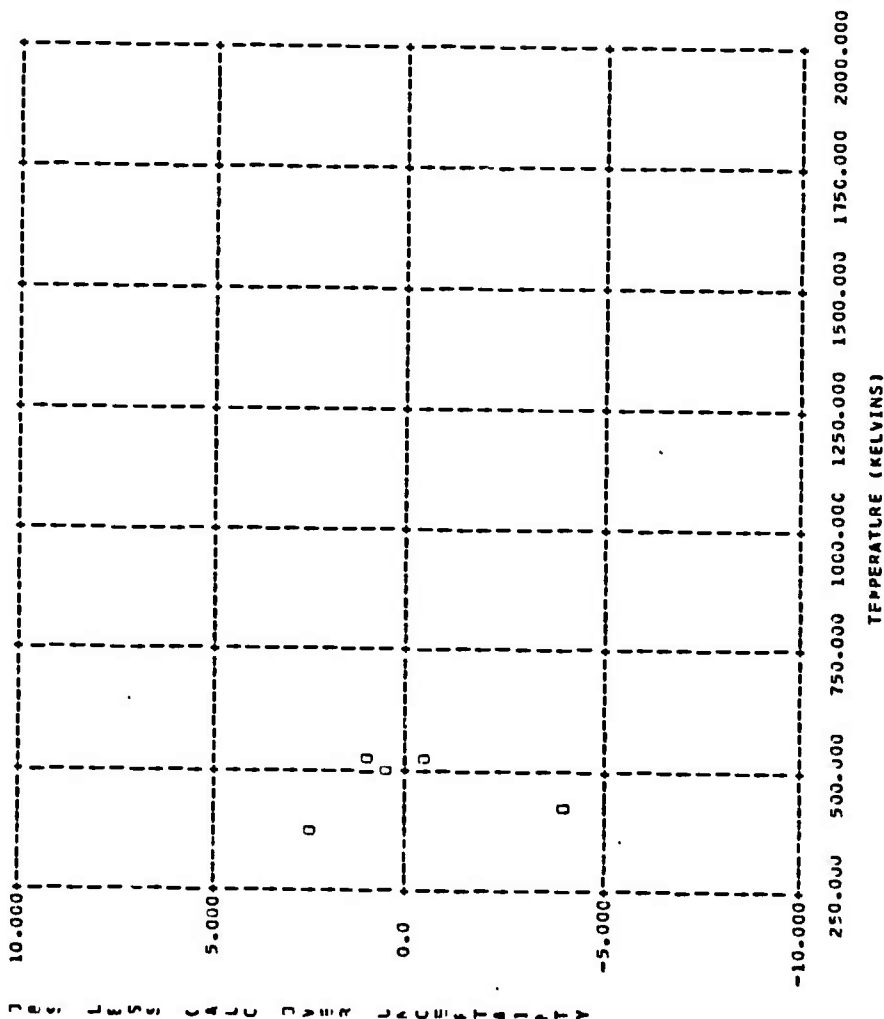
-----EL/TE/OT

BASE	CCCF	'A'/'G'	'B'	'C'	'D'	'E'	'F'
BUNSENIT	-1.000	2.27006860 C2 -2.62571050 C3	-1.62990600-01	8.55305780 C5	-9.81501070 C3	-1.49803830 C3	2.6514170-04
BUNSENIT	1.000	2.27006860 C2 -2.62571060 C3	-1.62550600-01	8.55305780 C5	-9.81501070 C3	-1.49803830 C3	2.6514170-04

13/31/73

FIGURE 2, THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

BUNSENITE, RELATIVE HEAT CONTENT. KING & CHRISTENSEN, JACS, 1958.



10/31/73

PROBLEM 2. THE SYSTEM MEAN AND THE THERMODYNAMICS OF BUNSENITE.

TEMPERATURE		T2-T1		FRFC	
T(2)	T(1)	OBSERVED	CALCULATED	PERCENT	OBS-CALC/SIGMO
VICKEL C210F, RELATIVE HEAT CONTENT KING AND CHRISTENSEN, JACS, 1958.					
535.500	298.150	3.08000 C3	3.07830 C3	0.3566	0.2829
544.600	298.150	3.20500 C3	3.20320 C3	0.0576	0.2880
554.200	298.150	3.33500 C3	3.33490 C3	0.0026	0.0130
556.200	298.150	3.34500 C3	3.36240 C3	-0.5191	-2.5554
561.200	298.150	3.44500 C3	3.43100 C3	0.4067	2.0336
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----					
				0.0039	0.0044
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE -----				0.2971	1.4856

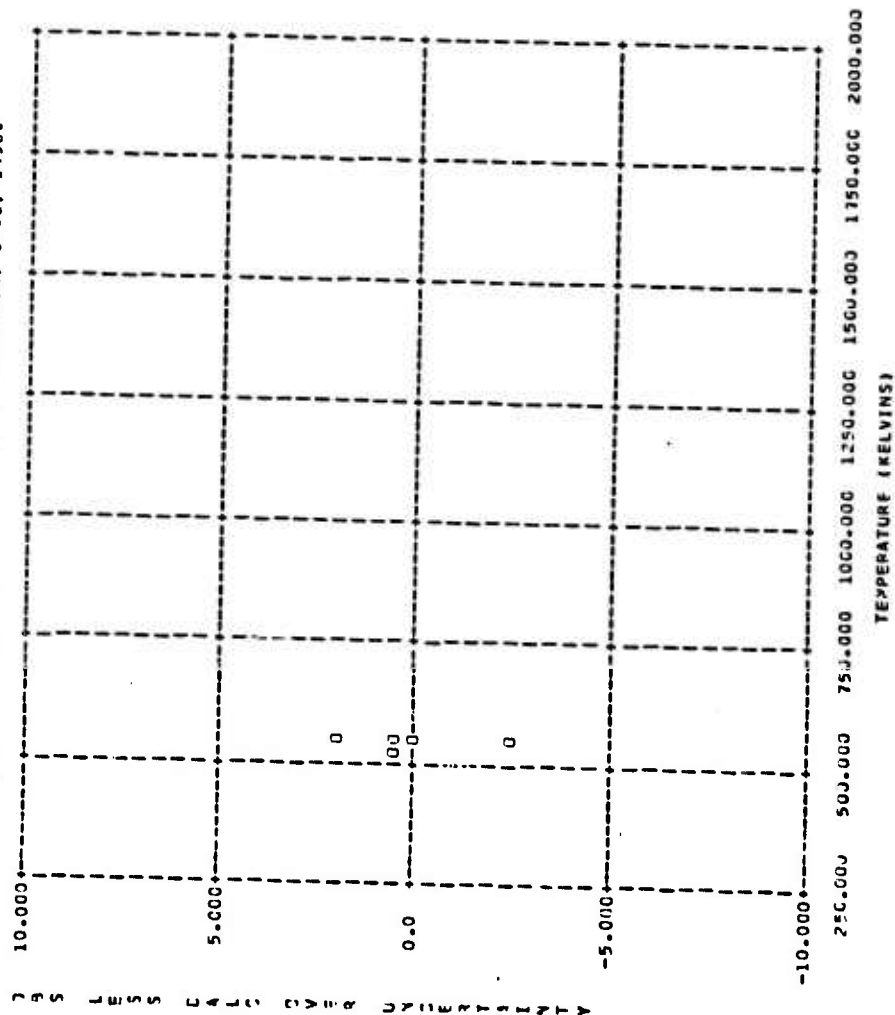
THE NUMBER OF OBSERVATIONS IS 5

10/31/73		T2-T1		FRFC	
BASE	COEF	A/V/G	B	C	D
VIC (B)	1.000	1.37249450 C1	0.0	0.0	0.0
BUNSENIT	-1.000	2.27006860 C2	-1.62550600-01	8.55305780 05	-1.49803830 03
		-2.62571060 C3			

12/31/73

PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

NICKEL OXIDE, RELATIVE HEAT CONTENT KING AND CHRISTENSEN, JACS, 1958.



PROBLEM 2, THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

TEMPERATURE		HT2-HT1		EPRC	
T(2)	T(1)	OBSERVED	CALCULATED	DIFFERENCE	PERCENT DRS-CALC/SIGMO
NICKEL OXIDE, RELATIVE HEAT CONTENT, KING AND CHRISTENSEN, JACS, 1958.					
572.300	298.150	3.58500 C3	3.58270 C3	2.2597	0.0630
672.300	298.150	4.86500 C3	4.87400 C3	-9.0317	-0.1856
765.700	298.150	6.31500 C3	6.31550 C3	-0.0419	-0.0066
872.300	298.150	7.44000 C3	7.44000 C3	0.0000	0.0000
944.500	298.150	8.62000 C3	8.62000 C3	0.0000	0.0000
1058.800	298.150	1.02100 C4	1.02150 C4	-5.0000	-0.0049
1206.500	298.150	1.17500 C4	1.17500 C4	0.0000	0.0000
1224.400	298.150	1.20200 C4	1.20210 C4	-0.0100	-0.0083
1304.300	298.150	1.31200 C4	1.31200 C4	0.0000	0.0000
1406.300	298.150	1.45400 C4	1.45220 C4	0.1800	0.0122
1500.500	298.150	1.58400 C4	1.58620 C4	-22.0000	-0.0139
1604.400	298.150	1.73000 C4	1.73610 C4	-61.0000	-0.0035
1706.800	298.150	1.88500 C4	1.88780 C4	-28.0000	-0.0015
1805.700	298.150	2.04400 C4	2.04370 C4	0.0300	0.0015

THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE -----

THE STANDARD DEVIATIONS ABOUT THE MEAN ARE -----

THE NUMBER OF OBSERVATIONS IS 14

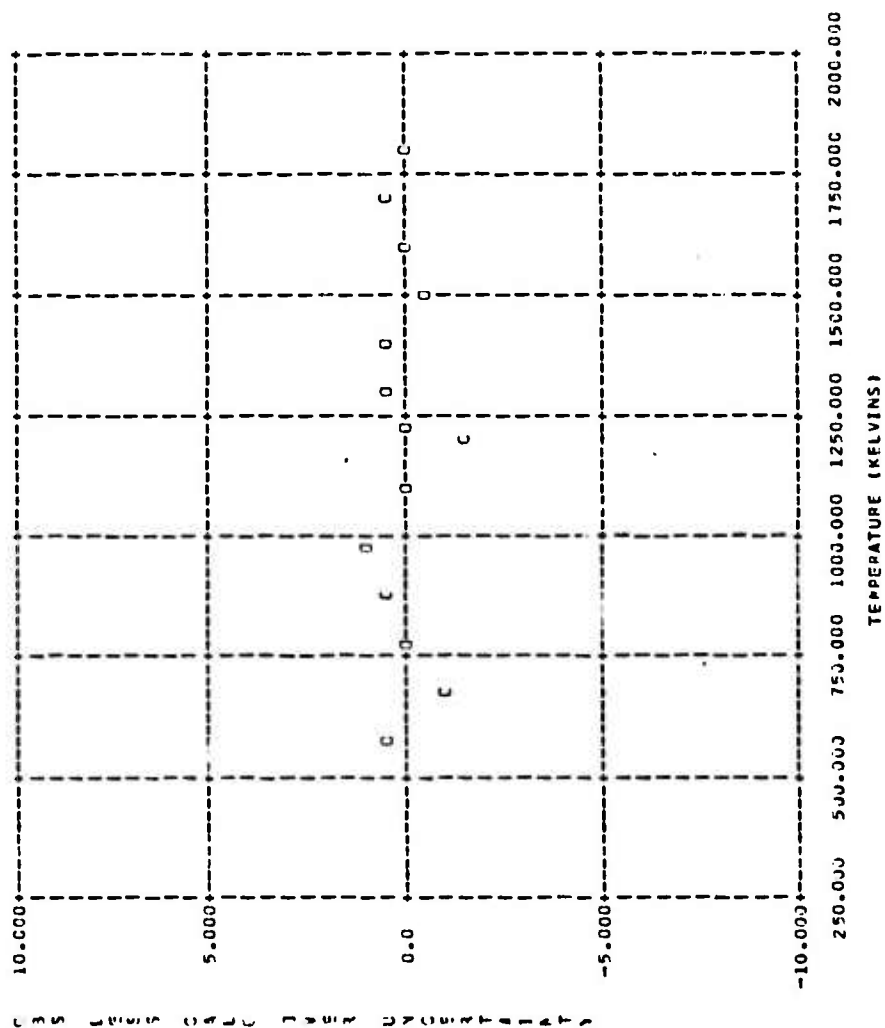
10/31/73-----

PHASE	CONF	'A'/'G'	'R'	'C'	'O'	'E'	'F'
ATC (C)	1.000	8.46856410 C0 0.0	1.82357740-03	8.36545000 C5	-4.82612510 C4	-3.71432740 C1	0.0
BUNSENIT	-1.000	2.27006860 C2 -2.62571060 C3	-1.62990600-01	8.55305780 C5	-9.81501070 C3	-1.49803830 C3	2.60914170-04

10/21/73

FIGURE 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

NICKEL OXIDE, RELATIVE HEAT CONTENT. KING AND CHRISTENSEN, JACS, 1958.



10/31/73

PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF EUNSENITE.

TEMPERATURE	ENTHALPY		ERROR	
	T(2)	T(1)	DIFFERENCE	PERCENT
EUNSENITE, HEAT OF FORMATION.				
			BOYLE, KING, AND CONWAY, 1954.	
298.150	0.0	-5.73000 04	-0.0000	-0.0000
THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE				
			-0.0000	-0.0000
THE STANDARD DEVIATIONS ABOUT THE MEAN ARE				
			0.0	0.0
THE NUMBER OF OBSERVATIONS IS				
				1

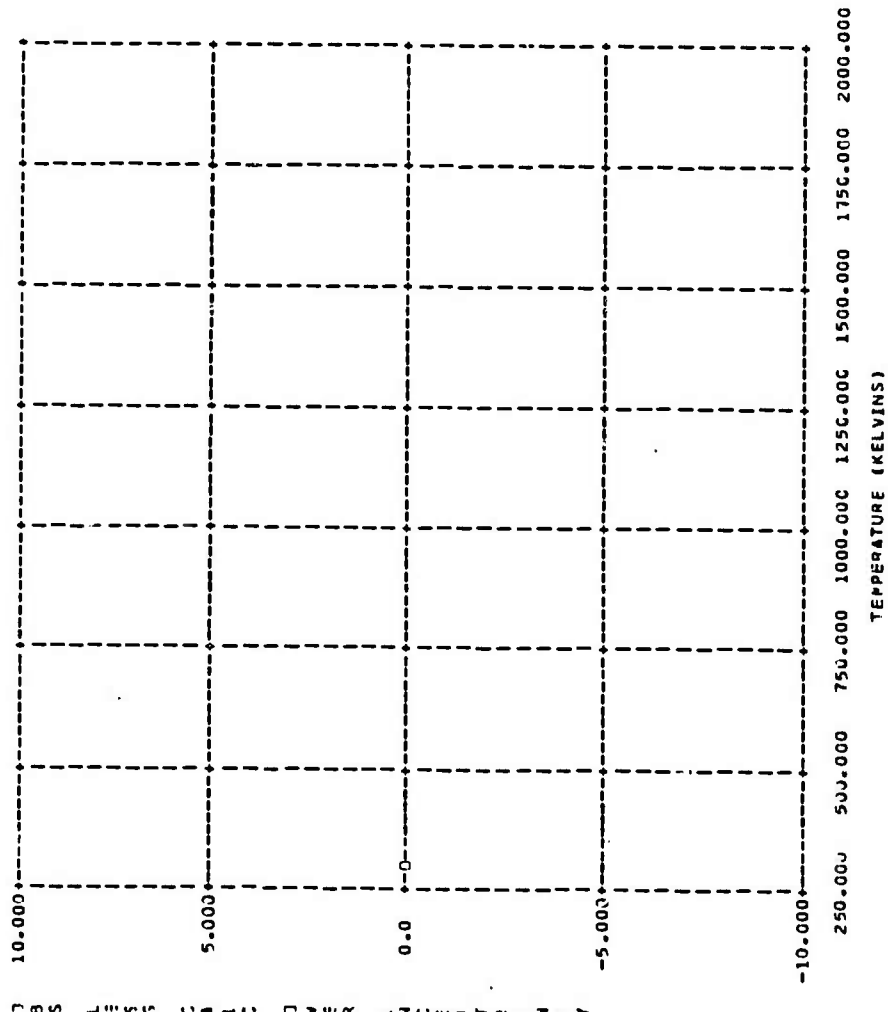
)C/31/73-----									
PHASE	CONF	'A'/'G'	'B'	'C'	'D'	'E'	'F'		
EUNSENIT	1.000	2.27036860 C2 -2.62571360 C-	-1.62590600-01	8.55305780 05	-9.81501070 03	-1.45803830 03	2.60914170-04		
NI (A)	-1.000	1.27036280 C1 C.C	-1.29019560-C2	-2.16220390 05	-1.79449530 03	-6.57710670 01	2.97703300-02		
12 (G)	-0.500	1.24086510 C1 -1.35520060 C2	-5.57401480-04	1.61901710 05	1.59013610 04	-4.18778890 01	2.50889120-07		
REACTION CONSTANTS									
		'A'/'G'	'B'	'C'	'D'	'E'	'F'		
		2.06598900 02 -2.55775050 C3	-1.45789540-01	9.90575320 05	-1.55711520 04	-1.41132820 03	2.31018390-04		

10/31/73

PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF RUNSENITE.

BOYLE, KING, AND GUNAW, 1954.

RUNSENITE, HEAT OF FORMATION.



THESE RESULTS WERE OBTAINED IN A PLN CN IC/31/73
 FACILEW 2, THE SYSTEM AI-C AND THE THERMODYNAMICS OF BUNSENITE.

AI (A)	HEAT CAP	ENTRCPY	ENTHALPY	GIBBS EN	LCG K	CELL EMF	T12-WT1
272.15	5.975	6.618	1980.	172.	-0.1378	-0.0075	-153.
298.15	6.224	7.153	2133.	0.	0.0000	0.0000	0.
400.00	6.794	9.069	2798.	-830.	0.4532	0.0360	666.
500.00	7.375	10.643	3505.	-1817.	0.7942	0.0788	1372.
600.00	8.338	12.067	4287.	-2553.	1.0757	0.1281	2144.
700.00	9.737	13.454	5189.	-4229.	1.3204	0.1834	3056.
800.00	11.776	14.885	6262.	-5646.	1.5423	0.2448	4130.
900.00	14.327	16.413	7563.	-7209.	1.7507	0.3126	5430.
1000.00	17.454	18.080	9147.	-8933.	1.9523	0.3874	7014.
1100.00	21.163	19.512	11073.	-10831.	2.1515	0.4697	8540.
1200.00	25.458	21.534	13399.	-12522.	2.3533	0.5603	11266.
1300.00	30.342	24.160	16184.	-15224.	2.5555	0.6602	14051.
1400.00	35.818	26.606	19487.	-17761.	2.7726	0.7702	17355.
1500.00	41.885	29.280	23367.	-20553.	2.9946	0.8913	21235.
1600.00	48.545	32.193	27834.	-23625.	3.2270	1.0245	25751.
1700.00	55.798	35.351	33096.	-27000.	3.4711	1.1708	30564.
1800.00	63.646	38.759	39063.	-30703.	3.7279	1.3314	36531.
1900.00	72.087	42.424	45845.	-34760.	3.9984	1.5073	42712.
2000.00	81.123	46.349	53501.	-39197.	4.2832	1.6957	51368.

1.37036200 J1 -1.29019560-C2 -2.16220390 05 -1.79449930 03 -6.57710670 J1 2.97703360-05 0-0

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73
 PROBLEM 2, THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

NI (B)	HEAT CAP	ENTROPY	ENTHALPY	GIBBS EN	LCC K	CELL EMF	PT2-PT1
273.15	20.092	2.866	-5771.	-6554.	5.2442	0.2842	-464.
298.15	17.195	4.495	-5307.	-6647.	4.8725	0.2882	0.
400.00	10.910	8.513	-3930.	-7335.	4.0077	0.3181	1377.
500.00	8.581	10.657	-2973.	-8302.	3.6287	0.3600	2334.
600.00	7.685	12.129	-2167.	-9445.	3.4403	0.4056	3140.
700.00	7.423	13.289	-1415.	-10717.	3.3461	0.4647	3842.
800.00	7.460	14.280	-673.	-12097.	3.3047	0.5246	4634.
900.00	7.637	15.168	81.	-13570.	3.2553	0.5884	5386.
1000.00	7.869	15.984	856.	-15128.	3.3063	0.6560	6163.
1100.00	8.108	16.746	1655.	-16765.	3.3309	0.7270	6967.
1200.00	8.326	17.461	2477.	-18476.	3.3649	0.8012	7784.
1300.00	8.504	18.135	3319.	-20256.	3.4053	0.8784	8626.
1400.00	8.632	18.770	4176.	-22101.	3.4502	0.9564	9483.
1500.00	8.699	19.368	5043.	-24009.	3.4960	1.0411	10350.
1600.00	8.732	19.930	5914.	-25974.	3.5479	1.1263	11231.
1700.00	8.636	20.456	6781.	-27993.	3.5988	1.2139	12089.
1800.00	8.498	20.946	7639.	-30064.	3.6502	1.3037	12946.
1900.00	8.285	21.400	8479.	-32181.	3.7017	1.3955	13786.
2000.00	7.997	21.818	9293.	-34343.	3.7528	1.4892	14600.
-3.10546550 JJ	6.81486260-03	1.47595540 06	0.0	2.66102410 J1	-4.13146690-06	0.0	
	'A'	'B'	'C'	'D'	'E'	'F'	'G'

THESE RESULTS WERE OBTAINED IN A RUN CN 10/31/73

PROBLEM 2. THE SYSTEM NI-O AND THE THERMODYNAMICS OF BUNSENITE.

HEAT CAP	ENTRCPY	ENTHALPY	GIBBS EN	LCG K	CELL EMP	F12-F11
273.15	8.178	-48119.	-50353.	40.2880	2.1835	-258.
298.15	9.080	-47862.	-50569.	37.0680	2.1928	0.
400.00	12.444	-46691.	-51669.	28.2306	2.2405	1170.
500.00	15.484	-45324.	-53066.	23.1950	2.3011	2578.
600.00	20.529	-43560.	-54771.	15.9504	2.3751	4302.
700.00	29.171	-41106.	-56822.	17.7405	2.4640	6756.
800.00	41.710	-37596.	-58292.	16.1977	2.5711	10266.
900.00	58.496	-32622.	-62285.	15.1248	2.7009	15240.
1000.00	79.763	-25747.	-65525.	14.4089	2.8589	22115.
1100.00	105.672	-16515.	-70373.	12.5818	3.0516	31347.
1200.00	136.342	-4454.	-75778.	13.8011	3.2860	42408.
1300.00	171.858	10915.	-82321.	13.8354	3.5657	56777.
1400.00	212.286	30081.	-90186.	14.0786	3.9108	77943.
1500.00	257.677	53538.	-95568.	14.5070	4.3176	101400.
1600.00	308.068	81783.	-110668.	15.1166	4.7985	125645.
1700.00	363.494	115319.	-123694.	15.5020	5.3638	163181.
1800.00	423.978	154651.	-138855.	16.8558	6.0214	232513.
1900.00	489.542	200284.	-156380.	17.9878	6.7811	248146.
2000.00	560.202	252725.	-176477.	19.2845	7.6526	300591.

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73
 PROBLEM 2. THE SYSTEM NI-C AND THE THERMODYNAMICS OF BUNSENITE.

NI-C (g)	HEAT CAP	ENTROPY	ENTHALPY	GIBBS FN	LCG K	CELL EMF	P12-M11
273.15	13.725	7.289	-48384.	-50375.	40.3058	2.1844	-343.
298.15	13.725	8.491	-48041.	-50573.	37.0708	2.1930	0.
400.00	13.725	12.525	-46643.	-51653.	28.2215	2.2399	1308.
500.00	13.725	15.587	-45271.	-53064.	23.1944	2.3010	2770.
600.00	13.725	18.090	-43898.	-54752.	19.9434	2.3742	4143.
700.00	13.725	20.205	-42526.	-56669.	17.6930	2.4574	5515.
800.00	13.725	22.038	-41153.	-58784.	16.0589	2.5491	6895.
900.00	13.725	23.655	-39781.	-61070.	14.8298	2.6482	8210.
1000.00	13.725	25.101	-38408.	-63505.	13.8759	2.7540	9633.
1100.00	13.725	26.409	-37036.	-66085.	13.1300	2.8657	11005.
1200.00	13.725	27.603	-35663.	-68787.	12.5278	2.9828	12378.
1300.00	13.725	28.702	-34291.	-71603.	12.0175	3.1049	13750.
1400.00	13.725	29.719	-32918.	-74525.	11.6338	3.2316	15123.
1500.00	13.725	30.666	-31546.	-77544.	11.2982	3.3626	16455.
1600.00	13.725	31.551	-30173.	-80656.	11.0170	3.4975	17868.
1700.00	13.725	32.384	-28801.	-83853.	10.7800	3.6361	19240.
1800.00	13.725	33.168	-27428.	-87131.	10.5751	3.7783	20613.
1900.00	13.725	33.910	-26056.	-90485.	10.4081	3.9237	21985.
2000.00	13.725	34.614	-24683.	-93912.	10.2622	4.0723	23358.
	'A'	'B'	'C'	'D'	'E'	'F'	'G'
1.27249450 J1	0.0	0.0	-5.21332130 04	-6.97078640 J1	0.0	0.0	0.0

THESE RESULTS WERE OBTAINED IN A RUN ON 10/31/73
 PROBLEM 2: THE SYSTEM NI-C AND THE THERMODYNAMICS OF RUNSENITE.

ATC (C)	HEAT CAP	ENTROPY	ENTHALPY	GIBBS EN	LCG K	CELL EMP	PT2-PT1
273.15	20.677	5.756	-48875.	-50447.	40.3629	2.1875	-405.
298.15	18.967	7.489	-48380.	-50613.	37.1003	2.1947	C.
400.00	15.156	12.441	-46673.	-51650.	28.2201	2.2397	1107.
500.00	13.639	15.636	-45244.	-53062.	23.1935	2.3010	9116.
600.00	12.981	18.056	-43918.	-54752.	19.5432	2.3742	4462.
700.00	12.729	20.035	-42635.	-56659.	17.6897	2.4569	5745.
800.00	12.694	21.731	-41265.	-58749.	16.0455	2.5476	7015.
900.00	12.785	23.230	-40092.	-60599.	14.8125	2.6451	8298.
1000.00	12.953	24.585	-38805.	-63390.	13.8540	2.7488	9575.
1100.00	13.173	25.830	-37499.	-65512.	13.0555	2.8582	10841.
1200.00	13.427	26.987	-36170.	-68553.	12.4853	2.9727	12210.
1300.00	13.706	28.072	-34813.	-71307.	11.9878	3.0921	13567.
1400.00	14.003	29.099	-33428.	-74166.	11.5778	3.2161	14952.
1500.00	14.312	30.075	-32012.	-77125.	11.2371	3.3444	16368.
1600.00	14.632	31.009	-30565.	-80180.	10.9520	3.4769	17815.
1700.00	14.960	31.906	-29085.	-83326.	10.7122	3.6133	19255.
1800.00	15.293	32.770	-27573.	-86560.	10.5098	3.7535	20807.
1900.00	15.631	33.606	-26027.	-89879.	10.3384	3.8974	22353.
2000.00	15.974	34.417	-24446.	-93280.	10.1932	4.0449	23934.

'A' 8.46856410 00
 'B' 1.0239774D-03
 'C' 8.2654980D 05
 'D' -4.8261251D 04
 'E' -3.7143274E 01
 'F' 0.0
 'G' 0.0

THESE RESULTS WERE OBTAINED IN A RUN CN 10/31/73

(C) 2

HEAT CAP	ENTRCPY	ENTHALPY	GIBBS EN	LCG K	CELL EMF	T-T-TI
273.15	7.047	14.336	1218.	-C.9742	-0.0528	-176.
298.15	7.024	14611.	-0.	-0.0000	0.0000	-0.
400.00	7.187	15333.	-5102.	2.7876	0.2212	722.
500.00	7.443	16064.	-10295.	4.4999	0.4464	147.
600.00	7.682	16821.	-15638.	5.6960	0.6781	2710.
700.00	7.888	17600.	-21105.	6.5904	0.9153	2985.
800.00	8.051	18398.	-26693.	7.2921	1.1575	3786.
900.00	8.206	19211.	-32378.	7.8623	1.4040	4600.
1000.00	8.328	20038.	-38154.	8.3385	1.6545	5427.
1100.00	8.434	20876.	-44013.	8.7447	1.9086	6265.
1200.00	8.525	21724.	-49950.	9.0971	2.1660	7112.
1300.00	8.605	22581.	-55957.	9.4073	2.4265	7960.
1400.00	8.678	23445.	-62031.	9.6835	2.6899	8814.
1500.00	8.743	24316.	-68167.	9.9319	2.9560	9705.
1600.00	8.804	25194.	-74361.	10.1573	3.2245	10562.
1700.00	8.862	26077.	-80610.	10.3632	3.4955	11466.
1800.00	8.917	26966.	-86912.	10.5525	3.7688	12355.
1900.00	8.971	27860.	-93263.	10.7276	4.0442	13249.
2000.00	9.024	28760.	-99661.	10.8904	4.3216	14145.

ATTACHMENT C

Listing of PHAS20 and Associated Routines

C	-----	PHA	10
C	PHAS20	PHA	20
C		PHA	30
C	THIS VERSION WILL HANDLE:	PHA	40
C		PHA	50
C	20 PHASES	PHA	60
C	70 DATA SETS	PHA	70
C	AND 1200 INDEPENDENT OBSERVATIONS.	PHA	80
C		PHA	90
C	VERSION TESTED 8/15/73 BY HAAS.	PHA	100
C	-----	PHA	110
C	IMPLICIT REAL*8(A-H,C-Z)	PHA	120
C	LOGICAL*1 LABEL, IMAGE, BCO	PHA	130
C	REAL*4 XMAX, XMIN, YMAX, YMIN, XI, E, TITLE, ACDEF, T, TO, AVAL, RELERR, SERR,	PHA	140
C	1 SERRSQ, EBAR, STDEV, ERR, AN	PHA	150
C	DIMENSION AVAL(7), SERR(3), SERRSQ(3), EBAR(3), STDEV(3), IMAGE(5000),	PHA	160
C	1 XI(1), E(1), PHINV(6), VAL(7), ION(20), IFMIN(20)	PHA	170
C	DIMENSION COEF(6,7), PNAME(20), TINV(6,70,4), IPHASE(6,70),	PHA	180
C	1 NPHASE(70), IKOUNT(70), IGO(70), ISTATE(6,70), NINVER(6,70),	PHA	190
C	2 INSTAT(6,70), INVPH(6,70,5), INVSC(6,70)	PHA	200
C	DIMENSION X(2,1200), YC(1200), SIGYO(1200), P(140), KI(140),	PHA	210
C	1 OC(140), PO(140), TITLE(20)	PHA	220
C	DIMENSION REF(10,70), ERRP(140), IHOLD(40)	PHA	230
C	DIMENSION SCINV(2), STCOEF(10), YESNO(2), TK(19,2), TYPE(14), NSCALE(5)	PHA	240
C	1 LABEL(50)	PHA	250
C	DIMENSION ODDC(7), OYOC(7)	PHA	260
C	DIMENSION AA(140)	PHA	270
C	-----	PHA	280
C	COMMON BLOCKS	PHA	290
C	NAME ROUTINES	PHA	300
C	EARTH MAIN PROGRAM, ORGLS2, EAFW20, PUTOUT	PHA	310
C	AIR MAIN PROGRAM, ORGLS2, TEST20, EAFW20	PHA	320
C	FIRE MAIN PROGRAM, ORGLS2, TEST20, EAFW20	PHA	330
C	WATER MAIN PROGRAM, EAFW20, YOERIV, ODERIV,	PHA	340
C	PUTOUT, FN, OIE, AND PLCKC DATA.	PHA	350
C	TIME MAIN PROGRAM, PUTOUT	PHA	360
C	SPACE MAIN PROGRAM, EAFW20, YOERIV, ODERIV,	PHA	370
C	AND PUTOUT	PHA	380
C	MAN MAIN PROGRAM, PUTOUT	PHA	390
C	-----	PHA	400
C	COMMON /EARTH/ COEF, PNAME, TINV, IPHASE, NPHASE, IKOUNT, IGO, NSETS,	PHA	410
C	1 ISTATE, NINVER, INSTAT, INVPH, INVSC, LISTP	PHA	420
C	COMMON /AIR/ X, P, OC, TITLE, YO, SIGYO, PO, KI, NC, NV, NX, IW,	PHA	430
C	1 NP, NO, ISING, ISTCP, IL, JN	PHA	440
C	COMMON /FIRE/ REF, ERRP, IWRITE, ICY, IICY, IRECC, IREG, NHOLD,	PHA	450
C	1 IHOLD	PHA	460
C	COMMON /WATER/ ZERC, ONE, TWO, THREE, FOUR, SIX, R, F,	PHA	470
C	1 SCINV, TREF, STCOEF, OIEO, ADIE, BCIE, THETA, YESNO, TK,	PHA	480
C	2 ASTAR, TYPE, NL, NSCALE, LABEL, BCO	PHA	490
C	COMMON /TIME/ OATE	PHA	500
C	COMMON /SPACE/ ODDC, OYOC, SC, TLOW	PHA	510
C	COMMON /MAN/ AA	PHA	520
C	EXTERNAL EAFW20	PHA	530
C	CALL ERRSET (208,256,C,2)	PHA	540
C	-----	PHA	550
C	READ IN AND STORE INPUT DATA--	PHA	560
C	OATE -- TODAY'S DATE	PHA	570
C	NREG -- NUMBER OF SEPARATE PROBLEMS IN THE DATA SET	PHA	580
C		PHA	590
C		PHA	600

C	-----	PHA 610
	READ (5,4400) OATE	PHA 620
	READ (5,4500) NREG	PHA 630
	00 4300 IREG=1,NREG	PHA 640
C	-----	PHA 650
C	INITIALIZE CONSTANTS	PHA 660
C	WRITE OATE	PHA 670
C	-----	PHA 680
	IICY=0	PHA 690
	KOUNT=J	PHA 700
	IWRITE=1	PHA 710
	WRITE (6,5300)	PHA 720
	WRITE (6,5400) OATE	PHA 730
C	-----	PHA 740
C	READ IN AND STORE --	PHA 750
C	TITLE (20) -- TITLE FOR CORRELATION	PHA 760
C	ID0 -- 1 FOR REGRESSION AND ERROR PLCTS	PHA 770
C	2 FOR REGRESSION ONLY	PHA 780
C	3 FOR ERROR PLOTS ONLY	PHA 790
C	NC -- NUMBER OF CYCLES. GENERALLY 2 IS SUFFICIENT.	PHA 800
C	SUBROUTINE TEST WILL TERMINATE REGRESSION	PHA 810
C	IF THE RELATIVE CHANGE IN SUCCESSIVE	PHA 820
C	PARAMETERS IS LESS THAN 1.00-8.	PHA 830
C	IW -- 0 FOR WEIGHTED DATA	PHA 840
C	1 FOR UNWEIGHTED DATA	PHA 850
C	IL -- 0 FOR CALCULATED RESULTS AT PLCT TIME ONLY	PHA 860
C	1 FOR CALCULATED RESULTS WITH EACH CYCLE	PHA 870
C	IFMOUT -- PUNCH F0PMAT FOR OUTPUT OF PARAMETERS--	PHA 880
C	0 GIVES PARAMETERS IN 6012.5 FORMAT	PHA 890
C	1 GIVES PARAMETERS IN 6A8 FORMAT.	PHA 900
C	LISTP -- NUMBER OF PHASES IN CORRELATION	PHA 910
C	ICY -- NUMBER OF STEPS IN STEP-BACKWARD ELIMINATION.	PHA 920
C	DEFAULT IS 0.	PHA 930
C	NHOLD -- NUMBER OF PARAMETERS TO BE KEPT WITHIN THE	PHA 940
C	REGRESSION EVEN THOUGH 'TEST' WILL INDICATE THEY ARE	PHA 950
C	NON-SIGNIFICANT.	PHA 960
C	PNAME(LISTP) -- 8-CHARACTER LABEL FOR EACH PHASE IN	PHA 970
C	CORRELATION	PHA 980
C	ION(LISTP) -- FLAG WHICH INDICATES THE SPECIES IS A	PHA 990
C	REFERENCE ELEMENT (1), A COMPOUND (0), OR AN ION (-1).	PHA1000
C	NSETS -- NUMBER OF DATA SETS IN CORRELATION	PHA1010
C	-----	PHA1020
	READ (5,4600) (TITLE(I),I=1,20)	PHA1030
	READ (5,4500) IOC,NC,IW,IL,IFMOUT	PHA1040
	READ (5,4500) LISTP,ICY,NHOLD	PHA1050
	READ (5,4400) (PNAME(M),M=1,LISTP)	PHA1060
	READ (5,4700) (ION(I),I=1,LISTP)	PHA1070
	READ (5,4500) NSETS	PHA1080
	WRITE (6,5500) (TITLE(I),I=1,20)	PHA1090
	WRITE (6,5600) (PNAME(M),M=1,LISTP)	PHA1100
	WRITE (6,5300)	PHA1110
	WRITE (6,5700) (TITLE(I),I=1,20),DATE	PHA1120
	WRITE (6,5800)	PHA1130
	PUNCH 4600, (TITLE(I),I=1,20)	PHA1140
	PUNCH 4500, LISTP	PHA1150
	PUNCH 4400, (PNAME(M),M=1,LISTP)	PHA1160
C	-----	PHA1170
C	READ IN AND STORE INPUT DATA FOR EACH DATA SET --	PHA1180
C	REF (10,J) -- REFERENCE FOR 'J' TH DATA SET (DATA SET	PHA1190
C	IDENTIFICATION)	PHA1200
C	NPHASE(J) -- NUMBER OF PHASES IN REACTION, SET TO 1 WHEN	PHA1210

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C          DATA FOR ONE PHASE ONLY.
C          IKOUNT(J) -- NUMBER OF OBSERVATIONS IN DATA SET
C          IGO(J) -- DATA TYPE,
C              FOR HEAT CAPACITY, IGO(J) IS 1
C              ENTROPY 2
C              ENTHALPY 3
C              GIBBS ENERGY 4
C              LOG(10) K 5
C              CELL DATA 6
C              DIFFERENTIAL HEAT,
C              H(T)-H(T0) 7
C          FOR ANY DATA NOT INCLUDED IN TYPES 1
C          THROUGH 7, SET IGO(J) TO ANY INTEGER
C          8 THRU 14. SUPPLY SUBROUTINE UNIQUE
C          TO CALCULATE YC (AND THE DERIVATIVES
C          OC(I) IF JN (OR JOFLAG) = ZERO) FROM
C          THE CURRENT VALUES OF THE PARAMETERS.
C          IF MORE THAN ONE TYPE OF DATA ARE TO BE
C          CONSIDERED, THESE ARE KEYED BY DIFFERENT
C          VALUES OF IGO(J).
C          ITFACT -- THE VALUES IS 1 IF TEMPERATURE IS IN KELVINS,
C          0 IF THE TEMPERATURE IS IN CENTIGRADE DEGREES.
C          IPARA -- PROGRAM IS SET FOR UNITS IN JCULES(*), VOLTS, OR
C          LOG(10)K IN MOLAL UNITS.
C          IF SO, SET IPARA TO 1
C          IF NOT, SET IPARA TO 0. PROGRAM MULTIPLIES YO(I) AND
C          SIGY(I) BY PARA TO BE READ LATER.
C          ISIG -- 0 IF WEIGHTS ARE RELATIVE.
C          1 IF WEIGHTS ARE ABSOLUTE.
C          (ABSOLUTE WEIGHTS ARE USED IN CALCULATIONS.)
C          (*) FOR DATA IN CALORIES, ADJUST R AND F IN BLOCK DATA. SEE
C          COMMENTS IN BLOCK DATA WHICH DESCRIBE THE NECESSARY
C          ADJUSTMENTS.
C          -----
C          DD 1800 J=1,NSETS
C          READ (5,4400) (REF(I,J),I=1,10)
C          WRITE (6,5900)
C          WRITE (6,6000) ASTAR
C          WRITE (6,5900)
C          WRITE (6,6100) J, (REF(I,J),I=1,10)
C          READ (5,4500) NPHASE(J),IKOUNT(J),IGO(J),ITFACT,IPARA,ISIG
C          WRITE (6,6200) NPHASE(J),IKCOUNT(J),TYPE(IGO(J))
C          NPPAS=NPHASE(J)
C          -----
C          FOR EACH DATA SET, READ AND STORE FOR ONE PHASE AT A TIME,
C          ANAME -- 8-CHARACTER PHASE LABEL. MUST BE THE SAME AS
C          GIVEN IN PNAME(LISTP).
C          COEF(I,J) -- COEFFICIENT IN REACTION (+1.000 IF NOT
C          REACTION)
C          ISTATE(I,J) -- FOR ELEMENTS IN LOWEST TEMPERATURE MODIFICA-
C          TION, SET TO 1
C          FOR COMPOUNDS AND ELEMENTS IN HIGHER TEMPER-
C          ATURE MODIFICATIONS, SET TO 0
C          NINVER(I,J) -- NUMBER OF INVERSIONS (EQUALS NUMBER OF LOWER
C          TEMPERATURE MODIFICATIONS BEING CONSIDERED
C          FOR COMPONENT.)
C          -----
C          DD 700 I=1,NPHAS
C          READ (5,4600) ANAME,COEF(I,J),ISTATE(I,J),NINVER(I,J)

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PHA1220
PHA1230
PHA1240
PHA1250
PHA1260
PHA1270
PHA1280
PHA1290
PHA1300
PHA1310
PHA1320
PHA1330
PHA1340
PHA1350
PHA1360
PHA1370
PHA1380
PHA1390
PHA1400
PHA1410
PHA1420
PHA1430
PHA1440
PHA1450
PHA1460
PHA1470
PHA1480
PHA1490
PHA1500
PHA1510
PHA1520
PHA1530
PHA1540
PHA1550
PHA1560
PHA1570
PHA1580
PHA1590
PHA1600
PHA1610
PHA1620
PHA1630
PHA1640
PHA1650
PHA1660
PHA1670
PHA1680
PHA1690
PHA1700
PHA1710
PHA1720
PHA1730
PHA1740
PHA1750
PHA1760
PHA1770
PHA1780
PHA1790
PHA1800
PHA1810
PHA1820

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C -----PHA1830
C LOCATE ANAME IN LIST PNAME(LISTP) AND ASSIGN THE INDEX TO PHA1840
C IPHASE(I,J). PHA1850
C -----PHA1860
C DO 100 K=I,LISTP PHA1870
C IF (ANAME.EQ.PNAME(K)) GO TO 200 PHA1880
100 CONTINUE PHA1890
C GO TO 4100 PHA1900
200 IPHASE(I,J)=K PHA1910
C NOYES=(ISTATE(I,J)+3)/2 PHA1920
C ACCEF=COEF(I,J) PHA1930
C WRITE (6,6300) PNAME(IPHASE(I,J)),ACCEF,YESAC(NYES),NINVER(I,J) PHA1940
C IF (NINVER(I,J).EQ.0) GO TO 700 PHA1950
C -----PHA1960
C IF (NINVER(I,J).GT.0) READ AND STORE, PHA1970
C INSTAT(I,J) -- FOR ELEMENTS, ASSIGN 1 PHA1980
C FOR COMPOUNDS, ASSIGN 0 PHA1990
C INVSC(I,J) -- IF UPON INVERSION THERE IS A STOICHIOMETRY PHA2000
C CHANGE (EG-- 2 FECL3 = FE2CL6), THEN FIND THE APPROPRIATE PHA2010
C REACTANT COEFFICIENT (HERE '2') IN THE VECTOR PHA2020
C STCOFF AND ENTER HERE. DEFAULT GIVES A COEFFICIENT OF PHA2030
C '1'. PHA2040
C TINVINVER(I,J) -- INVERSION TEMPERATURES, KELVINS PHA2050
C PHINV(NINVER(I,J)+1) -- PHASE NAME FOR ALL MODIFICATIONS, PHA2060
C BEGINNING WITH LOWEST TEMPERATURE MODIFICATION FIRST. NAME MUST CONFORM WITH NAMES PHA2070
C IN PNAME(LISTP). PHA2080
C PHA2090
C -----PHA2100
C KINVER=NINVER(I,J) PHA2110
C READ (5,4500) (TINV(I,J,K),K=1,KINVER) PHA2120
C KINVER=KINVER+1 PHA2130
C READ (5,5000) INSTAT(I,J),INVSC(I,J),(PHINV(K),K=1,KINVER) PHA2140
C IF (INVSC(I,J).EQ.0) INVSC(I,J)=1 PHA2150
C PHA2160
C LOCATE PHINV(NINVER(I,J)+1) IN LIST PNAME(LISTP) AND ASSIGN THE PHA2170
C INDEX TO INVPH(I,J). PHA2180
C -----PHA2190
C DO 500 K=I,KINVER PHA2200
C DO 300 L=I,LISTP PHA2210
C IF (PHINV(K).EQ.PNAME(L)) GO TO 400 PHA2220
300 CONTINUE PHA2230
C GO TO 4100 PHA2240
400 INVPH(I,J,K)=L PHA2250
500 CONTINUE PHA2260
C KINVER=KINVER-1 PHA2270
C WRITE (6,6400) PHA2280
C ACCEF=1.0 PHA2290
C DO 600 K=1,KINVER PHA2300
C IF (K.EQ.KINVER) ACCEF=STCOFF(INVSC(I,J)) PHA2310
C T=TINV(I,J,K) PHA2320
C WRITE (6,6500) ACCEF,PNAME(INVPH(I,J,K)),PNAME(INVPH(I,J,K+1)),T PHA2330
600 CONTINUE PHA2340
C IF (INSTAT(I,J).EQ.1) WRITE (6,6600) PNAME(INVPH(I,J,1)) PHA2350
700 CONTINUE PHA2360
C -----PHA2370
C INITIALIZE KO, KCUNT, AND IKOUNT(I). AFTER DATA IS STORED, PHA2380
C IKOUNT(I) CONTAINS THE LOCATION OF THE LAST ITEM IN THE PHA2390
C 'J' TH DATA SET. PHA2400
C -----PHA2410
C KO=KCUNT+1 PHA2420
C KCUNT=KOUNT+IKOUNT(J) PHA2430

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	IKCUNT(J)=KCUNT	PHA2440
	WRITE (6,6700)	PHA2450
	WRITE (6,6800) TYPE(IGC(J))	PHA2460
C	-----	PHA2470
C	READ AND STORE THE DATA IN THE J*TH DATA SET,	PHA2480
C	X(1,1) -- TEMPERATURE (SEE TFACT BELOW)	PHA2490
C	TFACT -- 0.000 IF TEMPERATURE IN KELVINS	PHA2500
C	273.1500 IF TEMPERATURE IN CENTIGRADE DEGREES	PHA2510
C	YO(1) -- DEFENDANT OBSERVATION	PHA2520
C	PARA -- CONVERSION FACTOR TO CONVERT DATA TO CALORIES OR	PHA2530
C	VOLTS (1.000 FOR DATA IN KILOCALORIES,	PHA2540
C	1.00-3 FOR DATA IN MILLIVOLTS, --OR THE	PHA2550
C	APPROPRIATE CONVERSION FACTOR FOR DATA IN	PHA2560
C	JOULES, BTU/LB, QUART*STONES/ACRE, ETC.)	PHA2570
C	SIGYC(1) -- SEE PROGRAM DESCRIPTION FOR ASSIGNING WEIGHTS.	PHA2580
C	X(2,1) -- FOR DATA TYPES (IGC(J)) FROM 1 THRU 6,	PHA2590
C	X(2,1) = ZERO.	PHA2600
C	FOR RELATIVE HEAT CONTENT DATA, X(2,1) IS THE BASE	PHA2610
C	TEMPERATURE. DEFAULT IS 298.15 K.	PHA2620
C	FOR DATA TYPES TO BE PROGRAMMED BY THE USER,	PHA2630
C	X(2,1) IS AN OPTIONAL SECOND INDEPENDENT	PHA2640
C	VAR(ABLL.	PHA2650
C	-----	PHA2660
C	DO 1700 I=K0,KCUNT	PHA2670
	READ (5,4500) X(1,1),TFACT,YO(1),PARA,SIGYC(1),X(2,1)	PHA2680
	IF ((IW.EQ.0).AND.(SIGYC(1).EQ.0.000).AND.(ISIG.EQ.0)) SIGYC(1)=(	PHA2690
	1000	PHA2700
	IF (ITFACT.EQ.1) GO TO 1000	PHA2710
C	-----	PHA2720
C	IF (TFACT = 0 X(1,1) = X(1,1) + TFACT	PHA2730
C	-----	PHA2740
	X(1,1)=X(1,1)+TFACT	PHA2750
	IF (IGC(J).EQ.7) GO TO 800	PHA2760
	X(2,1)=0.000	PHA2770
	GO TO 900	PHA2780
800	X(2,1)=X(2,1)+TFACT	PHA2790
900	CONTINUE	PHA2800
1000	CONTINUE	PHA2810
	IF (IPARA.EQ.1) GO TO 1100	PHA2820
C	-----	PHA2830
C	IF IPARA = 0 YO(1) = YO(1)*PARA	PHA2840
C	-----	PHA2850
	YO(1)=YO(1)*PARA	PHA2860
1100	CONTINUE	PHA2870
	IF (IW.EQ.1) GO TO 1300	PHA2880
	IF (ISIG.EQ.1) GO TO 1200	PHA2890
C	-----	PHA2900
C	IF ISIG = 0 SIGYC(1)= DABS (YO(1))*S(SIGYC(1))	PHA2910
C	-----	PHA2920
	SIGYC(1)=DABS(SIGYC(1)*YO(1))	PHA2930
	GO TO 1400	PHA2940
1200	CONTINUE	PHA2950
C	-----	PHA2960
C	IF IPARA = 0 SIGYC(1)=SIGYC(1)*PARA	PHA2970
C	-----	PHA2980
	IF (IPARA.EQ.0) SIGYC(1)=DABS(SIGYC(1)*PARA)	PHA2990
	GO TO 1400	PHA3000
1300	CONTINUE	PHA3010
	SIGYC(1)=DABS(YO(1)*1.00-2)	PHA3020
1400	CONTINUE	PHA3030
	IF (SIGYC(1).EQ.0.000) SIGYC(1)=1.000	PHA3040

IF I1IG01J).EQ.7).AND.IX(2,I).EQ.0.0001) X12,I)=258.1500	PHA3050
T=X11,I)	PHA3060
TC=X12,I)	PHA3070
IF ITO.NE.0.0) GO TO 1500	PHA3080
WRITE I6,6900) I,T,YO11),SIGYO11)	PHA3090
GO TC 1600	PHA3100
1500 CONTINUE	PHA3110
WRITE I6,7000) I,T,TO,YO11),SIGYO11)	PHA3120
1600 CONTINUE	PHA3130
1700 CONTINUE	PHA3140
1800 CONTINUE	PHA3150
WRITE I6,7100) IJ,IKCUNTIJ),J=1,NSETS)	PHA3160
C -----	PHA3170
C THE DATA HAS NOW BEEN STORED. INITIALIZE CONSTANTS NEEDED FOR	PHA3180
C CRGLE2.	PHA3190
C -----	PHA3200
NC=KCUNT	PHA3210
NP=LISTP*7	PHA3220
NX=2	PHA3230
I=0	PHA3240
C -----	PHA3250
C READ AND STORE,	PHA3260
C IFMIN -- INPLT FORMAT CFR PILISTP*7)	PHA3270
C 0 INDICATES I6G12.5/D12.5)	PHA3280
C 1 INDICATES (7A8)	PHA3290
C THE LATTER FORMAT HAS NO ROUNDOFF IN DATA TRANSFER.	PHA3300
C PILISTP*6) -- TRIAL PARAMETERS. IF VARIED, MAY NOT BE 0.000	PHA3310
C IF NOT VARIED, 0.000 OR A	PHA3320
C PREDETERMINED VALUE MAY BE USED	PHA3330
C KILISTP*6) -- 0 IF PARAMETER IS HELD CONSTANT.	PHA3340
C 1 IF PARAMETER IS TO BE VARIED	PHA3350
C I HOLD -- INDICES OF PARAMETERS IN PILISTP*7) WHICH ARE	PHA3360
C FORCED TO STAY IN REGRESSION DESPITE 'TEST' DETERMINA-	PHA3370
C TION THAT THESE PARAMETERS MAY BE NON-SIGNIFICANT.	PHA3380
C -----	PHA3390
C READ I5,5100) (IFMINII),I=1,LISTP)	PHA3400
C DO 2100 I=1,LISTP	PHA3410
C JO=1+7*I-1)	PHA3420
C JN=JC+6	PHA3430
C IF IIFMINII).EQ.1) GO TO 1900	PHA3440
C READ I5,4500) (PIJ),J=JO,JN)	PHA3450
C GO TO 2000	PHA3460
1900 CONTINUE	PHA3470
READ I5,4400) (PIJ),J=JO,JN)	PHA3480
2000 CONTINUE	PHA3490
DO 2100 J=JO,JN	PHA3500
AAIJ)=PIJ)	PHA3510
2100 CONTINUE	PHA3520
READ I5,5100) (KIIII),I=1,NP)	PHA3530
IF (NHOLD.NE.0) READ I5,4700) (IHOLCII),I=1,NHOLD)	PHA3540
C -----	PHA3550
C BYPASS REGRESSION IF ICC IS 3.	PHA3560
C -----	PHA3570
C IF I1DD.EC.3) GO TO 2600	PHA3580
2200 CONTINUE	PHA3590
NV=0	PHA3600
DO 2300 K=1,NP	PHA3610
IF (KIIK).EQ.0) GO TO 2300	PHA3620
NV=NK+1	PHA3630
2300 CONTINUE	PHA3640
JN=0	PHA3650

C	-----	PHA3660
C	ENTER DRGLS2 AND REFINER PARAMETERS	PHA3670
C	-----	PHA3680
C	CALL DRGLS2 (EAFW20)	PHA3690
C	IF (ISING.NE.0) GO TO 2600	PHA3700
C	-----	PHA3710
C	PUNCH REFINED PARAMETERS ON CARD, ONE PHASE AT A TIME AND INCLUDE	PHA3720
C	THE PHASE NAME ON THE CARD WITH THE RELATED PARAMETERS.	PHA3730
C	-----	PHA3740
C	DO 2500 I=1,LISTP	PHA3750
C	JC=1+7*(I-1)	PHA3760
C	IF (IFMDUT.EQ.1) GO TO 2400	PHA3770
C	JN=JC+5	PHA3780
C	PUNCH 8200, (P(J),J=JC,JN),PNAME(I)	PHA3790
C	JN=JN+1	PHA3800
C	PUNCH 8300, P(JN),DATE,PNAME(I)	PHA3810
C	GO TO 2500	PHA3820
C	2400 CONTINUE	PHA3830
C	JN=JC+6	PHA3840
C	PUNCH 8400, (P(J),J=JC,JN),DATE,PNAME(I)	PHA3850
C	2500 CONTINUE	PHA3860
C	IF (IDC.CC.2) GO TO 4000	PHA3870
C	2600 CONTINUE	PHA3880
C	IF (ICCY.CC.1) GO TO 2700	PHA3890
C	-----	PHA3900
C	SET UP AND PRINT ERROR PLOTS.	PHA3910
C	READ IN AND STORE	PHA3920
C	NHL -- NUMBER OF HORIZONTAL DIVISIONS ON ORDINATE LESS 1.	PHA3930
C	NSBH -- NUMBER OF HORIZONTAL LINES PER DIVISION.	PHA3940
C	NVL -- NUMBER OF VERTICAL DIVISIONS ON ABSCISSA LESS 1.	PHA3950
C	NSBV -- NUMBER OF VERTICAL LINES PER DIVISION.	PHA3960
C	XMAX -- MAXIMUM TEMPERATURE ON ABSCISSA.	PHA3970
C	XMIN -- MINIMUM TEMPERATURE ON ABSCISSA.	PHA3980
C	YMAX -- MAXIMUM ERROR ON ORDINATE.	PHA3990
C	YMIN = - YMAX.	PHA4000
C	-----	PHA4010
C	READ (5,4500) NHL,NSBH,NVL,NSBV	PHA4020
C	READ (5,5200) XMAX,XMIN,YMAX	PHA4030
C	YMIN=-YMAX	PHA4040
C	2700 CONTINUE	PHA4050
C	IF ((ISING.NE.0).AND.(IDC.NE.3)) GO TO 4200	PHA4060
C	IN=0	PHA4070
C	DO 3300 J=1,NSETS	PHA4080
C	WRITE (6,5300)	PHA4090
C	WRITE (6,5700) (TITLE(I),I=1,20),DATE	PHA4100
C	WRITE (6,7200) TYPE(IGO(J))	PHA4110
C	-----	PHA4120
C	INITIALIZE THE PLOT IMAGE.	PHA4130
C	-----	PHA4140
C	CALL PLOT1 (NSCALE,NHL,NSBH,NVL,NSBV)	PHA4150
C	CALL PLOT2 (IMAGE,XMAX,XMIN,YMAX,YMIN)	PHA4160
C	-----	PHA4170
C	INITIALIZE CONSTANTS AND COUNTERS.	PHA4180
C	-----	PHA4190
C	IC=IN+1	PHA4200
C	IN=IKOUNT(J)	PHA4210
C	DO 2800 I=1,3	PHA4220
C	SERR(I)=ZERO	PHA4230
C	SERRSQ(I)=ZERO	PHA4240
C	2800 CONTINUE	PHA4250
C	-----	PHA4260

C	CALCULATE AND PRINT YC. CALCULATE AND SUM THE DIFFERENCE (ERR),	PHA4270
C	PERCENT ERROR (RELERR), AND THE WEIGHTED DIFFERENCE (F).	PHA4280
C	-----	PHA4290
	DO 3100 I=10,IN	PHA4300
	CALL EAFW20 (YC,I)	PHA4310
	ERRDP=YU(I)-YC	PHA4320
	ERR=ERRDP	PHA4330
	IF (YU(I).EQ.ZERO) GO TO 2900	PHA4340
	RELERR=ERRDP*1.0C2/DABS(YU(I))	PHA4350
	GO TO 300C	PHA4360
2900	CONTINUE	PHA4370
	PELERR=ZERO	PHA4380
3000	CONTINUE	PHA4390
	F(I)=ERR/SIGYO(I)	PHA4400
	XI(I)=X(1,I)	PHA4410
	TC=X(2,I)	PHA4420
	WRITE (6,7300) XI(I),TC,YO(I),YC,ERR,RELERR,F(I)	PHA4430
C	-----	PHA4440
C	ENTER THE POINT ON THE PLOT IMAGE.	PHA4450
C	SUM THE ERRORS.	PHA4460
C	-----	PHA4470
	CALL PLOT2 (BCC,XI,E,I)	PHA4480
	SERR(1)=SERR(1)+ERR	PHA4490
	SERR(2)=SERR(2)+RELERR	PHA4500
	SERR(3)=SERR(3)+E(I)	PHA4510
	SERRSQ(1)=SERRSQ(1)+ERR*ERR	PHA4520
	SERRSQ(2)=SERRSQ(2)+RELERR*RELERR	PHA4530
	SERRSQ(3)=SERRSQ(3)+E(I)*E(I)	PHA4540
C	-----	PHA4550
C	CALCULATE AND WRITE THE STANDARD ERROR OF ESTIMATE FOR THE	PHA4560
C	DIFFERENCE, THE PERCENT ERROR, AND THE WEIGHTED DIFFERENCE.	PHA4570
C	-----	PHA4580
3100	CONTINUE	PHA4590
	NDATA=1+(IN-ID)	PHA4600
	AN=NCATA	PHA4610
	DO 3200 I=1,3	PHA4620
	EBAR(I)=SERR(I)/AN	PHA4630
	STDEV(I)=SQRT(SERRSQ(I)/AN-EBAR(I)*EBAR(I))	PHA4640
3200	CONTINUE	PHA4650
	WRITE (6,6700)	PHA4660
	WRITE (6,7400) (EBAR(I),I=1,3),(STDEV(I),I=1,3),NDATA	PHA4670
C	-----	PHA4680
C	CALL PUTOUT TO CALCULATE AND WRITE THE COMPLETE SET OF CONSTANTS	PHA4690
C	FOR TH PHASES AND FOR THE DATA SET. BYPASS THE LATTER SET	PHA4700
C	OF CONSTANTS IF IGO(J) IS GREATER THAN OR EQUAL TO 7 OR IF	PHA4710
C	THE J-TH DATA SET HAS ONLY ONE PHASE.	PHA4720
C	-----	PHA4730
	CALL PUTOUT (J)	PHA4740
C	-----	PHA4750
C	PRINT THE PLOT IMAGE FOR THE J-TH DATA SET.	PHA4760
C	-----	PHA4770
	WRITE (6,5300)	PHA4780
	WRITE (6,5700) (TITLE(I),I=1,20),DATE	PHA4790
	WRITE (6,7500) (REF(I,J),I=1,10)	PHA4800
	CALL PLOT4 (NL,LABEL)	PHA4810
	WRITE (6,7600)	PHA4820
3300	CONTINUE	PHA4830
C	-----	PHA4840
C	PUT OUT TABLES FOR EACH SPECIES IN THE LIST PNAME(LISTP).	PHA4850
C	-----	PHA4860
	SC=1.000	PHA4870

00 3900 L=1,LISTP	PHA4880
WRITE (6,5400) DATE	PHA4890
WRITE (6,5500) (TITLE(I),I=1,20)	PHA4900
WRITE (6,7700) PNAME(L)	PHA4910
WRITE (6,7800) (TYPE(I),I=1,7)	PHA4920
INDEX=1+7*(L-1)	PHA4930
KOUNT=19	PHA4940
IF (IDJ(L).EQ.-1) KOUNT=15	PHA4950
M=(ICN(L)+4)/2	PHA4960
DO 3800 K=1,KOUNT	PHA4970
T=TK(K,M)	PHA4980
DO 3600 J=1,7	PHA4990
VAL(J)=0.000	PHA5000
IGDES=J	PHA5010
IF (IDJ(L).EQ.-1) IGDES=IGDES+7	PHA5020
IF (IGDES.EQ.14) GO TO 3600	PHA5030
CALL YDERIV (TK(K,M),IGDES)	PHA5040
DO 3400 I=1,7	PHA5050
VAL(J)=VAL(J)+OYDC(I)*AA(INDEX+I-1)	PHA5060
3400 CONTINUE	PHA5070
IF (J.NE.7) GO TO 3600	PHA5080
CALL YDERIV (298.1500,J)	PHA5090
OC 3500 I=1,7	PHA5100
VAL(J)=VAL(J)-OYDC(I)*AA(INDEX+I-1)	PHA5110
3500 CONTINUE	PHA5120
3600 CONTINUE	PHA5130
DO 3700 I=1,7	PHA5140
AVAL(I)=VAL(I)	PHA5150
3700 CONTINUE	PHA5160
WRITE (6,7900) T,(AVAL(I),I=1,7)	PHA5170
3800 CONTINUE	PHA5180
JO=INDEX	PHA5190
JN=JC+6	PHA5200
WRITE (6,8700)	PHA5210
WRITE (6,8000) (AA(J),J=JO,JN)	PHA5220
PUNCH 8500, (AA(J),J=JO,JN),PNAME(L),DATE	PHA5230
3900 CONTINUE	PHA5240
IF (IDJ.EC.3) GO TO 4200	PHA5250
C -----	PHA5260
C IF STEP-BACKWARD ELIMINATION OF NON-SIGNIFICANT PARAMETERS IS	PHA5270
C IN EFFECT (ICY.NE.U), SET LEAST SIGNIFICANT PARAMETER TO	PHA5280
C ZERO AND REPEAT REGRESSION.	PHA5290
C -----	PHA5300
4000 IF ((IREDC.EQ.0).CR.(ICY.GT.ICY)) GO TO 4200	PHA5310
KI(IREDC)=0	PHA5320
P(IREDC)=0.000	PHA5330
ICY=ICY+1	PHA5340
GO TO 2200	PHA5350
4100 CONTINUE	PHA5360
WRITE (6,8100) J	PHA5370
4200 CONTINUE	PHA5380
4300 CONTINUE	PHA5390
STOP	PHA5400
C -----	PHA5410
C FORMAT STATEMENTS	PHA5420
C -----	PHA5430
4400 FORMAT (1CA8)	PHA5440
4500 FORMAT (1E15)	PHA5450
4600 FORMAT (2CA4)	PHA5460
4700 FORMAT (4CI2)	PHA5470
4800 FORMAT (A8,2X,010.3,10X,2I5)	PHA5480

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4900 FORMAT (6C12.5) PHA5490
5000 FORMAT (15,13,9A8/(1CA8)) PHA5500
5100 FORMAT (8C11) PHA5510
5200 FORMAT (8E10.3) PHA5520
5300 FORMAT (1F1) PHA5530
5400 FORMAT (42H1 THESE RESULTS WERE OBTAINED IN A RUN ON ,A8) PHA5540
5500 FORMAT (1F0,20A4/1H0) PHA5550
5600 FORMAT (6CH0 PHASES CONSIDERED IN THIS REGRESSION ARE AS FOLLOWS PHA5560
1WS---/1H0,10X,5A2C/(1H ,10X,5A20)) PHA5570
5700 FORMAT (1F ,20A4,40X,A8/1H0) PHA5580
5800 FORMAT (54H0THE FOLLOWING DATA SETS HAVE BEEN READ IN TO STORAGE:/PHA5590
11H0SET NUMBER,10X,9HREFERENCE) PHA5600
5900 FORMAT (1F0) PHA5610
6000 FORMAT (1F ,A8) PHA5620
6100 FORMAT (1F ,16,14X,10A8) PHA5630
6200 FORMAT (25H0THE NUMBER OF PHASES IS:,10/31H THE NUMBER OF OBSERVATPHA5640
1ICNS IS:,15/21H THE TYPE OF DATA IS:,3X,A8/11H0PHASE NAME,10X,11HCPHA5650
20EFFICIENT,9X,10HREF. STATE,10X,10HINVERSIONS/1H ) PHA5660
6300 FORMAT (1F ,1X,A8,11X,F8.3,15X,A3,14X,16) PHA5670
6400 FORMAT (1F0,10X,26HINVERSIONS ARE AS FOLLOWS:/1H ) PHA5680
6500 FORMAT (1H ,F15.2,3X,A8,5X,1H=,5X,A8,F20.3) PHA5690
6600 FORMAT (1F0,10X,A8,5X,58HIS A REFERENCE PHASE AND HAS ZERO Gibbs Enthalpy PHA5700
1ENERGY AT 298.15 K/1H0) PHA5710
6700 FORMAT (1F ) PHA5720
6800 FORMAT (1H ,15X,5HINDEX,21X,11HTEMPERATURE,18X,A8,13X,5HERROR/1H ,PHA5730
135X,2HT2,18X,2HT1/1H ) PHA5740
6900 FORMAT (1F ,120,F20.3,16X,1H=,3X,1P20.5) PHA5750
7000 FORMAT (1H ,120,2F20.3,1P20.5) PHA5760
7100 FORMAT (92H1THE INDEX OF THE LAST ITEM OF THE ABOVE DATA SETS IN TPHA5770
1HE VECTORS X(1,1), Y(1,1), AND SIGY(1)/15H IS AS FOLLOWS:/1H0,30X,PHA5780
28HCATA SET,3X,5HINDEX//1H ,24X,2110)) PHA5790
7200 FORMAT (1H ,9X,11HTEMPERATURE,20X,A8,30X,5HERROR/1H ,9X,11H-----PHA5800
1-----,20X,8H-----,22X,21H-----/1H ,7X,4HT(2),8X,PHA5810
24HT(1),9X,8HOBERVED,8X,10HCALCULATED,6X,10HDIFFERENCE,4X,7HPERCENTPHA5820
3T,2X,14HCBS-CALC/SIGY) PHA5830
7300 FORMAT (1H ,2F12.3,1P20.5,4OP3F13.4) PHA5840
7400 FORMAT (55H0THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET ARE ---PHA5850
1--- ,3F13.4/59H0THE STANDARD DEVIATIONS ABOUT THE MEAN ARE -----PHA5860
2----- ,2F13.4/31H0THE NUMBER OF OBSERVATIONS IS ,15) PHA5870
7500 FORMAT (1H0,10A8/1H ) PHA5880
7600 FORMAT (1H0,T35,21HTEMPERATURE (KELVINS)) PHA5890
7700 FORMAT (1H0/1H ,A8/1H0) PHA5900
7800 FORMAT (1H ,15X,A8,8X,A8,8X,A8,8X,A8,8X,A8,8X,A8,8X,A8/1H ) PHA5910
7900 FORMAT (1H0,F7.2,2F16.3,2F16.0,2F16.4,F16.0) PHA5920
8000 FORMAT (1H0,10X,3H'A',15X,3H'B',15X,3H'C',15X,3H'D',15X,3H'E',15X,3H'F',15X,3H'G'/1H0,1P7D18.7) PHA5930
8100 FORMAT (35H I,YOUR FRIENDLY COMPUTER, DO NOW CUIT./5H0IN YOUR ,14,PHA5940
146H1THE DATA SET YOU HAVE MISSTYPED THE PHASE NAME.) PHA5950
8200 FORMAT (1F0C12.5,A8) PHA5960
8300 FORMAT (1P1012.5,52X,2A8) PHA5970
8400 FORMAT (7A8,8X,2A8) PHA5980
8500 FORMAT (7A8,8HCOMPLETE,2A8) PHA5990
END PHA6000
PHA6010-

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BLOCK DATA
IMPLICIT REAL*8(A-H,C-Z)
LOGICAL*1 BCC,LABEL
DIMENSION SCINV(2),STODEF(101),YESNO(2),TK(19,21),TYPE(14),NSCALE(51)
1 ,LABEL(50)
-----
COMMON BLOCKS
NAME RDUTINES
EARTH MAIN PROGRAM, DRCLS2, EAFW20, PUTOUT
AIR MAIN PROGRAM, DRCLS2, TEST20, EAFW20
FIRE PUTOUT AND UNICL.
WATER MAIN PROGRAM, DRCLS2, TEST20, EAFW20
TIME MAIN PROGRAM, EAFW20, YDERIV, ODERIV,
SPACE PUTOUT, FV, DIF, AND BLOCK DATA.
MAN MAIN PROGRAM, PLTCLT
-----
COMMON /JCOLES/UNITS
COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, F,
1 SCINV, TREF, STODEF, DIEO, A, B, THETA, YESNO, TK,
2 ASTAR, TYPE, NL, NSCALE, LABEL, BCC
-----
THE FOLLOWING VALUES OF 'R' AND 'F' ARE TO BE USED FOR ENERGY
DATA IN CALORIES.
DATA R,F/4.575616500,2.306094604/
THE FOLLOWING VALUES OF 'R' AND 'F' ARE TO BE USED FOR ENERGY
DATA IN JOULES.
DATA R,F/19.14437500,9.64870004/
-----
DATA L'HITS/OF JOULES /
DATA R,F/19.14437500,9.64870004/
DATA ZERO,ONE,TWO,THREE,FOUR,SIX/0.000,1.000,2.000,3.000,4.000,
1 6.000/
DATA SCINV/-1.000,1.000/
DATA TREF/2.981502/
DATA STODEF /1.000,2.000,3.000,4.000,5.000,0.500,0.400,0.33333333
13300,0.2500,0.200/
DATA DIEO,A,B,THETA/3.05702,1.8750-2,-1.274101,2.1902/
DATA YESNO /3HNO,3HYES/
DATA TYPE /8HHEAT CAP,8HENTROPY,8HENTHALPY,8HGI88S EN,
1 8HLOG K,8HCELL EMP,8HHT2-HT1,7*8HSPECIAL /
DATA ASTAR/8H*****/
DATA TK /273.1500,298.1500,323.1500,349.1500,373.1500,398.1500,
1 423.1500,448.1500,473.1500,498.1500,523.1500,548.1500,573.1500,
2 598.1500,623.1500,0.000,0.000,0.000,0.000,273.1500,298.1500,
3 4.002,5.002,6.002,7.002,8.002,9.002,1.003,1.103,1.203,1.303,
4 1.403,1.503,1.603,1.703,1.803,1.903,2.003/
DATA LABEL /30HUBS LESS CALC OVER UNCERTAINTY/
DATA NL/30/
DATA BCC/1+0/
DATA NSCALE/5*0/
END

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C   FORMAT STATEMENTS
100 FORMAT (1F120A4)
200 FORMAT (32HNUMBER OF CYCLES IN THIS JOB ISI2/37HNUMBER OF PARAMETERS TO BE VARIED ISI3/51HNUMBER OF INDEPENDENT VARIABLES PER OBSERVATION ISI2)
300 FORMAT (46HDERIVATIVES PROGRAMMED IN SUBROUTINE EAFW20. )
400 FORMAT (31HWEIGHTS TO BE SUPPLIED BY USER)
500 FORMAT (34HUNIT WEIGHTS TO BE SET BY PROGRAM)
600 FORMAT (25HNUMBER OF PARAMETERS READ ISI4)
700 FORMAT (31HNUMBER OF OBSERVATIONS READ ISI5)
800 FORMAT (46HOCALCULATED Y BASED ON PARAMETERS BEFORE CYCLEI2)
900 FORMAT (1F0,10X,5FINDEX,7X,4HT(2),8X,4HT(1),10X,6HY(D8S),10X,7HY(CORR)
1000 FORMAT (1F ,I15,F12.3,12X,1P4016.3,OPF16.4)
1100 FORMAT (1F ,I15,2F12.3,1P4016.3,OPF16.4)
1200 FORMAT (1F ,I15,F12.3,12X,5F16.4)
1300 FORMAT (1F ,I15,2F12.3,5F16.4)
1400 FORMAT (51HAGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLEI2/2CRG
1500 FORMAT (6CHBESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS AFTER CYCLEI2/2CHOSUM(W*(O-C)**2) IS 011.3/35HQSRTF(SUM(W*(O-C)**2)/(NC-NV)) IS 2010.4)
1600 FORMAT (62H MATRIX HAS A ZERO DIAGONAL ELEMENT CORRESPONDING TO PARAMETERI3,16H OF THOSE VARIED)
1700 FORMAT (4CH SINGULARITY RETURN FROM MATRIX INVERTER)
1800 FORMAT (37HOPARAMETERS AFTER LEAST SQUARES CYCLEI2/1H0,T16,'OLD',TORG
1900 FORMAT (1F0,A8)
2000 FORMAT (1F 13,2(4X,1PD17.10))
2100 FORMAT (1F ,I3,1P5021.10,OPF17.4)
2200 FORMAT (66HOSUBROUTINE TEST INDICATES THAT JOB IS TO BE TERMINATEDORC
2300 FORMAT (16HOTRIAL CONSTANTS/1H0,2X,1HI,9X,4HP(I),6X,5HKI(I)/1H )
2400 FORMAT (1F0,9X,A8)
2500 FORMAT (1F ,I3,5X,1PC11.4,6X,I1)
2600 FORMAT (15HOCORRELATION MATRIX)
2700 FORMAT (1F0I3,100I2.4/(1H 3X,100I2.4))
2800 FORMAT (14H1***WARNING***93HOTHER TERM SIG/(NC-NV) IS NEGATIVE. THE ABSOLUTE VALUE IS TAKEN AND THE REGRESSION CONTINUES.)
2900 CONTINUE
WRITE (6,100) (TITLE(I),I=1,20)
WRITE (6,200) NC,NV,NX
WRITE (6,300)
IF (IW) 3100,3000,3100
3000 WRITE (6,400)
GO TO 3200
3100 WRITE (6,500)
3200 CONTINUE
WRITE (6,600) NP
WRITE (6,700) NC
IF (NC) 3300,3300,3500
3300 GO 3400 I=1,NP
3400 KI(I)=0
C   INITIALIZE PROBLEM AND ENTER SUBROUTINE PRELIM IF PROVIDED
3500 NM=(NV*(NV+1))/2
SQSIG(1)=C.000
CALL PRELIM

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C	PUT OUT TPIAL PARAMETERS, AND KEY-INTEGERS.	CRG1220
	WRITE (6,2300)	CRG1230
	JO=1	CRG1240
	DO 3600 I=1,LISTP	CRG1250
	WRITE (6,2400) PNAME(I)	CRG1260
	JN=JC+6	CRG1270
	WRITE (6,2500) (J,P(I),KI(I),J=JC,JN)	CRG1280
	JO=JC+7	CRG1290
3600	CONTINUE	CRG1300
C	START LOOP TO PERFORM NC CYCLES AND ONE FINAL CALCULATION OF Y	CRG1310
	NCY=NC+1	CRG1320
	DO 7900 IC=1,NCY	CRG1330
C	CLEAR ARRAYS AM AND V EXCEPT ON LAST CYCLE	CRG1340
	IF (IC=NCY) 3700,4000,4000	CRG1350
3700	DO 3800 I=1,NM	CRG1360
3800	AM(I)=0.000	CRG1370
	DO 3900 I=1,NV	CRG1380
3900	V(I)=0.000	CRG1390
C	INITIALIZE FOR CYCLE IC AND PUT OUT CAPTION FOR LIST OF Y(CALC)	CRG1400
4000	SIG(2)=SIG(1)	CRG1410
	SIG=0.000	CRG1420
	WRITE (6,100) (TITLE(I),I=1,20)	CRG1430
	IF (IL.NE.0) GO TO 4100	CRG1440
	IF (IC.NE.NCY) GO TO 4200	CRG1450
4100	CONTINUE	CRG1460
	WRITE (6,800) IC	CRG1470
	WRITE (6,900)	CRG1480
4200	CONTINUE	CRG1490
C	START LOOP THROUGH NO OBSERVATIONS	CRG1500
	DO 5900 I=1,NO	CRG1510
C	ENTER USER'S SUBROUTINE TO COMPUTE Y(CALC) AND DERIVATIVES	CRG1520
	CALL CALC (YC,I)	CRG1530
C	OBTAIN WEIGHT AND CALCULATE QUANTITIES FROM Y(OBS)-Y(CALC)	CRG1540
	IF (IW) 4400,4300,4400	CRG1550
4300	SQRTW=1.000/SIGYC(I)	CRG1560
	GO TO 4500	CRG1570
4400	SIGYO(I)=1.000	CRG1580
	SQRTW=1.000	CRG1590
4500	DY=YC(I)-YC	CRG1600
	WDY=SQRTW*DY	CRG1610
	SIG=SIG+WDY*WDY	CRG1620
C	PUT OUT Y(CALC) AND OTHER INFORMATION FOR ONE OBSERVATION	CRG1630
	IF (IL.NE.0) GO TO 4600	CRG1640
	IF (IC.NE.NCY) GO TO 5100	CRG1650
4600	CONTINUE	CRG1660
	OUT(1)=X(1,I)	CRG1670
	OUT(2)=X(2,I)	CRG1680
	OUT(3)=YO(I)	CRG1690
	OUT(4)=YC	CRG1700
	OUT(5)=DY	CRG1710
	OUT(6)=SIGYO(I)	CRG1720
	OUT(7)=WDY	CRG1730
	IF (X(2,I).EQ.C.000) GO TO 4800	CRG1740
	IF ((DABS(YC(I)).LT.1.00-3).AND.(YO(I).NE.0.000)) GO TO 4700	CRG1750
	WRITE (6,1300) I,(OUT(K),K=1,7)	CRG1760
	GO TO 5000	CRG1770
4700	CONTINUE	CRG1780
	WRITE (6,1100) I,OUT(1),OUT(2),YO(I),YC,CY,SIGYC(I),OUT(7)	CRG1790
	GO TO 5000	CRG1800
4800	CONTINUE	CRG1810
	IF ((DABS(YO(I)).LT.1.00-3).AND.(YO(I).NE.0.000)) GO TO 4900	CRG1820

WRITE (6,1200) I,CUT(1),(OUT(K),K=3,7)	ORG1830
GO TO 500C	ORG1840
4900 CONTINUE	ORG1850
WRITE (6,1000) I,CUT(1),YD(1),YC,DY,SIGYC(1),OUT(7)	ORG1860
5000 CONTINUE	ORG1870
5100 CONTINUE	ORG1880
C BY-PASS DERIVATIVE AND MATRIX SET-UP ON FINAL CALC OF Y	ORG1890
IF (IC-NCY) 5200,5900,5900	ORG1900
C START LOOP TO STORE AN ARRAY OF NV DERIVATIVES	ORG1910
5200 J=1	ORG1920
DO 5400 K=1,NP	ORG1930
IF (KI(K)) 5400,5400,5300	ORG1940
5300 CONTINUE	ORG1950
C OBTAIN DERIVATIVE FROM THOSE PROGRAMMED BY USER	ORG1960
DV(J)=SQRTW*OC(K)	ORG1970
J=J+1	ORG1980
5400 CONTINUE	ORG1990
C END LOOP TO OBTAIN DERIVATIVES	ORG2000
C START LOOP TO STORE MATRIX AND VECTOR.	ORG2010
C 1604 CR GLS STORAGE SCHEME IS REVERSE OF 7090 CR GLS	ORG2020
JK=1	ORG2030
DO 5800 J=1,NV	ORG2040
TEMP=OV(J)	ORG2050
IF (TEMP) 5600,5500,5600	ORG2060
C BY-PASS IF DERIVATIVE IS ZERO	ORG2070
5500 JK=JK+NV+1-J	ORG2080
GO TO 5800	ORG2090
5600 DO 5700 K=J,NV	ORG2100
AM(JK)=AM(JK)+TEMP*OV(K)	ORG2110
JK=JK+1	ORG2120
5700 CONTINUE	ORG2130
V(J)=V(J)+TEMP*WDY	ORG2140
5800 CONTINUE	ORG2150
C END LOOP TO STORE MATRIX AND VECTOR	ORG2160
5900 CONTINUE	ORG2170
C END LOOP THROUGH NO OBSERVATIONS	ORG2180
C COMPUTE AND PUT OUT AGREEMENT FACTORS	ORG2190
CNVN=NP-NV	ORG2200
SQSIG(1)=CSQRT(SIG/(CNVN))	ORG2210
WRITE (6,1400) IC,SIG,SQSIG(1)	ORG2220
C BY-PASS MATRIX INVERSION AND PARAMETER OUTPUT ON FINAL CYCLE	ORG2230
IF (IC-NCY) 6000,8000,8000	ORG2240
C START LOOP TO TEST FOR ZERO DIAGONAL ELEMENT	ORG2250
6000 ISING=0	ORG2260
II=1	ORG2270
IIO=NV	ORG2280
DO 6300 I=1,NV	ORG2290
IF (AM(II)) 6200,6100,6200	ORG2300
6100 ISING=1	ORG2310
WRITE (6,1600) I	ORG2320
6200 II=II+IIO	ORG2330
IIC=IIO-1	ORG2340
6300 CONTINUE	ORG2350
C END LOOP TO TEST FOR ZERO DIAGONAL ELEMENT	ORG2360
C TERMINATE JOB IF ZERO DIAGONAL ELEMENT WAS FOUND	ORG2370
IF (ISING) 8600,6400,8600	ORG2380
C ENTER SUBROUTINE TO REPLACE MATRIX WITH INVERSE	ORG2390
6400 CALL MINVZG (AM,NV,ISING)	ORG2400
IF (ISING) 6500,6600,6500	ORG2410
C TERMINATE JOB IF SINGULAR MATRIX WAS FOUND	ORG2420
6500 WRITE (6,1700)	ORG2430

GO TO 8600	ORG2440
C START LOOP FOR MATRIX VECTOR MULTIPLICATION FOR	ORG2450
C PARAMETER CHANGES	ORG2460
6600 DO 7100 I=1,NV	ORG2470
PCI=0.000	ORG2480
IJ=I	ORG2490
IJO=NV-1	ORG2500
DO 7000 J=1,NV	ORG2510
POI=POI+AM(IJ)*V(J)	ORG2520
IF (J-I) 6700,6800,6900	ORG2530
6700 IJ=IJ+JJO	ORG2540
IJC=IJO-1	ORG2550
GO TO 7000	ORG2560
C SAVE DIAGONAL ELEMENTS OF INVERSE MATRIX	ORG2570
6800 DIAG(I)=AM(IJ)	ORG2580
6900 IJ=IJ+1	ORG2590
7000 CONTINUE	ORG2600
POI=POI	ORG2610
SIG=SIG-PCI*V(I)	ORG2620
7100 CONTINUE	ORG2630
C END LOOP FOR MATRIX VECTOR MULTIPLICATION	ORG2640
C RECOMPUTE AGREEMENT FACTOR USING MODIFIED SIG	ORG2650
IF (SIG) 7200,7300,7300	ORG2660
7200 CONTINUE	ORG2670
WRITE (6,2800)	ORG2680
SIG=DAES(SIG)	ORG2690
7300 CONTINUE	ORG2700
SCSIG(I)=DSQRT(SIG/(NV-1))	ORG2710
C PUT OUT CAPTION FOR LIST OF CORRECTED PARAMETERS	ORG2720
WRITE (6,100) (TITLE(I),I=1,20)	ORG2730
WRITE (6,1800) IC	ORG2740
C START LOOP TO CORRECT AND PUT OUT PARAMETERS	ORG2750
J=1	ORG2760
JO=1	ORG2770
DO 7700 IC=1,LISTP	ORG2780
WRITE (6,1900) PNAME(IC)	ORG2790
JN=JC+6	ORG2800
DO 7600 I=JO,JN	ORG2810
IF (KI(I)) 7400,7400,7500	ORG2820
7400 WRITE (6,2000) I,P(I),P(I)	ORG2830
GO TO 7600	ORG2840
7500 POLO=P(I)	ORG2850
P(I)=POLO+PC(I)	ORG2860
SIGP=DSQRT(DIAG(J))*SCSIG(I)	ORG2870
PCTCHG=1.02*PO(J)/P(I)	ORG2880
PCTERR=DAES(1.002*SIGP/P(I))	ORG2890
ERRP(I)=PCTERR	ORG2900
WRITE (6,2100) I,POLO,PD(J),P(I),SIGP,PCTCHG,PCTERR	ORG2910
J=J+1	ORG2920
7600 CONTINUE	ORG2930
JO=JO+7	ORG2940
7700 CONTINUE	ORG2950
C END LOOP TO CORRECT AND PUT OUT PARAMETERS	ORG2960
C PUT OUT ESTIMATED AGREEMENT FACTORS	ORG2970
WRITE (6,1500) IC,SIG,SCSIG(I)	ORG2980
C ENTER USERS SUBROUTINE TO TEST AND MODIFY PARAMETERS	ORG2990
C OR END JOB	ORG3000
ISTOP=0	ORG3010
CALL TEST20	ORG3020
C TERMINATE JOB IF INDICATED BY USERS SUBROUTINE TEST	ORG3030
IF (ISTOP) 7800,7900,7800	ORG3040

7800	WRITE (6,2200) 1STOP	ORG3050
	GO TO 8000	ORG3060
7900	CONTINUE	ORG3070
C	END LOOP THROUGH NC CYCLES AND FINAL CALC OF Y	ORG3080
C	TERMINATE JOB	ORG3090
8000	IF (NC) 8600,8600,8100	ORG3100
C	CALCULATE AND PUT OUT CORRELATION MATRIX	ORG3110
8100	WRITE (6,100) (TITLE(I),I=1,20)	ORG3120
	WRITE (6,2600)	ORG3130
	DO 8200 I=1,NV	ORG3140
	DIAG(I)=1.000/DSQRT(DIAG(I))	ORG3150
8200	CONTINUE	ORG3160
	IJ=1	ORG3170
	DO 8500 I=1,NV	ORG3180
	DO 8300 J=1,NV	ORG3190
	RCW(J)=J.CC0	ORG3200
8300	CONTINUE	ORG3210
	DO 8400 J=1,NV	ORG3220
	R0W(J)=AM(IJ)*DIAG(I)*DIAG(J)	ORG3230
	IJ=IJ+1	ORG3240
8400	CONTINUE	ORG3250
	WRITE (6,2700) I,(RCW(J),J=1,NV)	ORG3260
8500	CONTINUE	ORG3270
8600	CONTINUE	ORG3280
	RETURN	ORG3290
	END	ORG3300-

C	SUBROUTINE PRELIM	PRE 001
C	-----	PRE 002
C	CALL SUBROUTINE PRELIM	PRE 003
C	-----	PRE 004
	RETURN	PRE 005
	END	PRE 006

	SUBROUTINE TEST20	YES 10
C	-----	YES 20
C		TFS 30
C	TEST20	TFS 40
C		TFS 50
C	TEST20 TERMINATES THE REGRESSION IF THE CHANGE IN ALL	TFS 60
C	PARAMETERS IS LESS THAN 1.0D-8.	TFS 70
C		TFS 80
C	TEST20 WILL ALSO CAUSE IREDO TO TAKE THE INDEX OF THE	TFS 90
C	PARAMETER WHICH HAS THE GREATEST ERROR, PROVIDED ICY HAS	TFS 100
C	AN NON-ZERO VALUE AND PROVIDED THE ERROR ON ONE OR MORE	TFS 110
C	PARAMETERS IS GREATER THAN 10 PERCENT.	TFS 120
C		TFS 130
C	-----	TFS 140
C	IMPLICIT REAL*8 (A-H,C-Z)	TFS 150
C	REAL*4 TITLE	TFS 160
C	DIMENSION X(2,1200),YC(1200),SIGYO(1200),P(140),KI(140),	TFS 170
C	1 DC(140),PD(140),TITLE(20)	TFS 180
C	DIMENSION REF(10,70),ERRP(140),IHOLD(40)	TFS 190
C	-----	TFS 200
C	COMMON BLOCKS	TFS 210
C	NAME ROUTINES	TFS 220
C	EARTH MAIN PROGRAM, ORCLS2, EAFW20, PUTOUT	TFS 230
C	AIR MAIN PROGRAM, ORCLS2, TEST20, EAFW20	TFS 240
C	PUTOUT AND UNICL.	TFS 250
C	FIRE MAIN PROGRAM, ORCLS2, TEST20, EAFW20	TFS 260
C	WATER MAIN PROGRAM, EAFW20, YCERIV, ODERIV,	TFS 270
C	PUTOUT, FN, DIF, AND PLOCK DATA.	TFS 280
C	TIME MAIN PROGRAM, PLTOUT	TFS 290
C	SPACE MAIN PROGRAM, EAFW20, YCERIV, ODERIV,	TFS 300
C	AND PUTOUT	TFS 310
C	MAN MAIN PROGRAM, PLTOUT	TFS 320
C	-----	TFS 330
C	COMMON /AIR/ X, P, DC, TITLE, YC, SIGYO, FC, KI, NC, NV, NX, IW,	TFS 340
C	1 NP, NO, ISING, ISTOP, IL, JOFLAG	TFS 350
C	COMMON /FIRE/ REF, ERRP, IWRITE, ICY, IICY, IREDO, IREG, NHOLD,	TFS 360
C	1 IHOLD	TFS 370
C	IREDO=0	TFS 380
C	ISTAY=0	TFS 390
C	J=1	TFS 400
C	DO 400 I=1,NP	TFS 410
C	IF (KI(I).EQ.0) GO TO 400	TFS 420
C	IF (DABS(PD(I)/P(I)).GT.1.0D-8) ISTAY=1	TFS 430
C	J=J+1	TFS 440
C	IF (ICY.EQ.0) GO TO 400	TFS 450
C	DERAP=ERRP(I)	TFS 460
C	IF (DERAP.LE.1.0D1) GO TO 400	TFS 470
C	IF (IREDO.EQ.0) GO TO 100	TFS 480
C	IF (DERAP.LE.ERRP(IREDO)) GO TO 400	TFS 490
C	100 CONTINUE	TFS 500
C	IF (NHOLD.EQ.0) GO TO 300	TFS 510
C	DO 200 K=1,NHOLD	TFS 520
C	IF (I.EQ.IHOLD(K)) GO TO 400	TFS 530
C	200 CONTINUE	TFS 540
C	300 CONTINUE	TFS 550
C	IREDO=1	TFS 560
C	400 CONTINUE	TFS 570
C	IF (ISTAY.EQ.1) GO TO 500	TFS 580
C	ISTJP=1	TFS 590
C	500 RETURN	TFS 600

END

TFS 610-

SUBROUTINE MINV20 (AM,N,NFAIL)	MIN 10
IMPLICIT REAL*8(A-H,C-Z)	MIN 20
DIMENSION AM(10010)	MIN 30
C ***** SEGMENT 1 OF CHOLSKI INVERSION *****	MIN 40
C ***** FACTOR MATRIX INTO LOWER TRIANGLE X TRANSPSE *****	MIN 50
K=1	MIN 60
IF (N-1) 100,200,300	MIN 70
100 NFAIL=K	MIN 80
GO TO 200C	MIN 90
200 AM(1)=1.0/AM(1)	MIN 100
GO TO 190C	MIN 110
C ***** LOCF M OF A(L,M) *****	MIN 120
300 DO 120J M=1,N	MIN 130
IMAX=M-1	MIN 140
C ***** LOCF L OF A(L,M) *****	MIN 150
DO 110J L=M,N	MIN 160
SUMA=0.0	MIN 170
KLI=L	MIN 180
KMI=M	MIN 190
IF (IMAX) 600,600,400	MIN 200
C *****SUM OVER I=1,M-1 A(L,I)*A(M,I) *****	MIN 210
400 DO 50J I=1,IMAX	MIN 220
SUMA=SUMA+AM(KLI)*AM(KMI)	MIN 230
J=A-I	MIN 240
KLI=KLI+J	MIN 250
500 KMI=KMI+J	MIN 260
C *****TERM=C(L,M)-SUM *****	MIN 270
600 TERM=AM(K)-SUMA	MIN 280
IF (L-M) 700,700,1000	MIN 290
700 IF (TERM) 900,900,900	MIN 300
C ***** A(M,M)=SQRT(TERM) *****	MIN 310
800 DENCM=DSQRT(TERM)	MIN 320
AM(K)=DENCM	MIN 330
GO TO 110C	MIN 340
900 NFAIL=K	MIN 350
GO TO 200C	MIN 360
C ***** A(L,M)=TERM/A(M,M) *****	MIN 370
1000 AM(K)=TERM/DENCM	MIN 380
1100 K=K+1	MIN 390
1200 CONTINUE	MIN 400
C ***** SEGMENT 2 OF CHOLSKI INVERSION *****	MIN 410
C *****INVERSION OF TRIANGULAR MATRIX*****	MIN 420
AM(1)=1.0/AM(1)	MIN 430
KOM=1	MIN 440
C ***** STEP L OF B(L,M) *****	MIN 450
DO 150J L=2,N	MIN 460
KOM=KOM+N-L+2	MIN 470
C ***** RECIPROCAL CF DIAGONAL TERM *****	MIN 480
TER=1.0/AM(KOM)	MIN 490
AM(KM)=TERM	MIN 500
KMI=0	MIN 510
KLI=L	MIN 520
IMAX=L-1	MIN 530
C ***** STEP M OF B(L,M) *****	MIN 540
DO 140J M=1,IMAX	MIN 550
K=KLI	MIN 560
C ***** SUM TERMS *****	MIN 570
SUMA=0.0	MIN 580
DO 130J I=M,IMAX	MIN 590
II=KMI+I	MIN 600

SUM A=SUM A-AM(KLI)*AM(II)	MIN 610
1300 KLI=KLI+N-I	MIN 620
C ***** MULT SUM * RECIP OF DIAGNAL *****	MIN 630
AM(K)=SUM A*TERM	MIN 640
J=N-M	MIN 650
KLI=K+J	MIN 660
1400 KM I=KM I+J	MIN 670
1500 CONTINUE	MIN 680
C ***** SEGMENT 3 OF CHOLESKI INVERSION *****	MIN 690
C *****PREMULTIPLY LOWER TRIANGLE BY TRANSFCSE*****	MIN 700
K=1	MIN 710
DO 1800 M=1,N	MIN 720
KLI=K	MIN 730
DO 1700 L=M,N	MIN 740
KM I=K	MIN 750
IMAX=N-L+1	MIN 760
SUM A=0.0	MIN 770
DO 1600 I=1,IMAX	MIN 780
SUM A=SUM A+AM(KLI)*AM(KM I)	MIN 790
KLI=KLI+1	MIN 800
1600 KM I=KM I+1	MIN 810
AM(K)=SUM A	MIN 820
1700 K=K+1	MIN 830
1800 CONTINUE	MIN 840
1900 NFAIL=0	MIN 850
2000 RETURN	MIN 860
END	MIN 870-

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C      SUBROUTINE EAFW20 (YC,I)
C      -----
C      EAFW20
C      THIS VERSION WRITTEN 3/09/72 BY HAAS.
C      LAST MODIFIED 8/05/72 BY HAAS.
C      -----
C      IMPLICIT REAL*8(A-H,C-Z)
C      LOGICAL*1 BCC,LABEL
C      REAL*4 TITLE
C      DIMENSION SGN(2)
C      DIMENSION CCEF(6,70),PNAME(20),TINV(6,70,4),IPHASE(6,70),
1  NPHASE(70),IKOUNT(70),IGD(70),ISTATE(6,70),NINVER(6,70),
2  INSTAT(6,70),INVPH(6,70,5),INVSC(6,70)
C      DIMENSION X(3,1200),YC(1200),SIGYC(1200),P(140),KI(140),
1  DC(140),PD(140),TITLE(20)
C      DIMENSION REF(10,70),ERRP(140),IHOLD(40)
C      DIMENSION SCINV(2),STCDEF(10),YESN(2),TK(19,2),TYPL(14),NSCALE(5)
1  ,LABEL(50)
C      DIMENSION DCCC(7),DYDC(7)
C      -----
C      COMMON PLCKCS
C      NAME          ROUTINES
C      EARTH          MAIN PROGRAM, ORGLS2, EAFW20, PUTCLT
C      AIR            MAIN PROGRAM, ORGLS2, TEST20, EAFW20
C      FIRE           MAIN PROGRAM, ORGLS2, TEST20, EAFW20
C      WATER          MAIN PROGRAM, EAFW20, YDERIV, CDERIV,
C      TIME           PUTOUT, FN, DIS, AND PLCKC DATA.
C      SPACE          MAIN PROGRAM, EAFW20, YDERIV, CDERIV,
C      MAN            AND PUTOUT
C      PLTOUT         MAIN PROGRAM, PLTOUT
C      -----
C      COMMON /EARTH/ CCEF,PNAME,TINV,IPHASE,NPHASE,IKOUNT,IGD,NSETS,
1  ISTATE,NINVER,INSTAT,INVPH,INVSC,LISTP
C      COMMON /AIR/ X, P, DC, TITLE, YC, SIGYC, PD, KI, AC, NV, NX, IW,
1  NP, NJ, ISING, ISTOP, IL, JDFLAG
C      COMMON /FIRE/ REF,ERRP,WRITE,ICY,IICY,IRED,IREG,NHOLD,
1  IHOLD
C      COMMON /WATER/ ZERD, CNE, TWO, THREE, FOUR, SIX, R, F,
1  SCINV, TRFF, STCDEF, DIED, ADIE, BDIE, THETA, YESN, TK,
2  ASTAR, TYPE, NI, NSCALE, LABEL, BCC
C      COMMON /SPACE/ DCCC, DYDC, SC, TO
C      YC=ZERO
C      DO 100 K=1,NP
C      CCK(K)=ZERD
100 CONTINUE
C      DETERMINE J BY LOCATING I IN THE VECTOR IKOUNT. IF NOT
C      LOCATED, PRINT ERROR MESSAGE AND STOP
C      -----
C      DO 200 J=1,NSETS
C      IF (I.LS.IKOUNT(J)) GO TO 300
200 CONTINUE
C      WRITE (6,2000)
C      STCP
300 CONTINUE

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C -----EAF 610
C WRITE REFERENCE IF THE 1-TH OBSERVATION IS THE FIRST IN THE EAF 620
C J-TH DATA SET. EAF 630
C -----EAF 640
C IF (IWRITE.EQ.1.OR.I.EQ.1) GO TO 400 EAF 650
C GO TO 500 EAF 660
400 CONTINUE EAF 670
WRITE (6,2100) (REF(I,J,I,1)=1,101 EAF 680
IWRITE=J EAF 690
500 CONTINUE EAF 700
IF (I.EQ.IKOUNT(J)) IWRITE=J EAF 710
IF (IGO(J).LE.7) GO TO 600 EAF 720
C -----EAF 730
C IF IGC(J) IS GREATER THAN 7, CALL UNIQUE TO CALCULATE EAF 740
C YC (AND THE DERIVATIVES DC(III IF JCFLAG (JN IN PHAS20) IS EAF 750
C ZFRJ. EAF 760
C -----EAF 770
C CALL UNIQUE (YC,I,J,JFLAG) EAF 780
C RETURN EAF 790
600 CONTINUE EAF 800
C -----EAF 810
C FOR EACH PHASE IN THE J-TH DATA SET, CALCULATE THE SEVEN EAF 820
C DERIVATIVES. EAF 830
C -----EAF 840
C T=X(1,I) EAF 850
C TC=X(2,I) EAF 860
C LAST=NPHASE(J) EAF 870
C DO 1800 L=1, LAST EAF 880
C -----EAF 890
C LOCATE THE FIRST CONSTANT FOR THE L-TH PHASE IN THE VECTOR P. EAF 900
C INITIALIZE SC, THE STOICHIOMETRIC COEFFICIENT. EAF 910
C -----EAF 920
C INDEX=1+7*(IPHASE(L,J)-1) EAF 930
C SC=CCOF(L,J) EAF 940
C -----EAF 950
C CALL YDERIV TO CALCULATE THE TEMPERATURE TERM IN THE DERIVATIVE. EAF 960
C IF THE DATA SET IS FOR ENTROPY AND HEAT CAPACITY, GO TO EAF 970
C STATEMENT 130. EAF 980
C -----EAF 990
C IGCES=IGO(J) EAF1000
C IF (ISTATE(L,J).EQ.-1) IGCES=IGCES+7 EAF1010
C CALL YDERIV (T,IGCES) EAF1020
C IF (IGO(J).LE.2) GO TO 1600 EAF1030
C -----EAF1040
C CALL ODERIV TO CALCULATE THE DERIVATIVE WITH RESPECT TO -C- AT EAF1050
C 298.15 KELVIN IF COMPONENT IS AN ELEMENT. PROCEED TO ADJUST EAF1060
C GO ACCORDINGLY. EAF1070
C -----EAF1080
C IF (ISTATE(L,J).NE.1) GO TO 600 EAF1090
C CALL ODERIV (TREF) EAF1100
C DO 700 K=1,7 EAF1110
C DC(K+INDEX)-1=DC(K+INDEX)-1+SC*ODOC(K)*OYCC(4) EAF1120
700 CONTINUE EAF1130
GO TO 1600 EAF1140
800 CONTINUE EAF1150
C -----EAF1160
C CHECK FOR INVERSIONS. IF LOW TEMPERATURE PHASES ARE TO BE EAF1170
C CONSIDERED, INITIALIZE SGN. IF LOW TEMPERATURE PHASES EAF1180
C ARE NOT TO BE CONSIDERED, GO TO STATEMENT 130. EAF1190
C -----EAF1200
C IF (NINVER(L,J).LE.0) GO TO 1600 EAF1210

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DO 900 LLL=1,2	FAF1220
SGN(LLL)=SCINV(LLL)	FAF1230
900 CONTINUE	FAF1240
IF (INVSC(L,J).EQ.0) GO TO 1000	FAF1250
SGN(1)=SGN(1)*STCCEF(INVSC(L,J))	FAF1260
SGN(2)=SGN(2)*STCCEF(INVSC(L,J))	FAF1270
1000 CONTINUE	FAF1280
C -----	FAF1290
C IF THE LOWEST TEMPERATURE PHASE IS AN ELEMENT, CALL DDERIV	FAF1300
C THE ARGUMENT IS 298.15, AND PROCEED TO ADJUST DC	FAF1310
C ACCORDINGLY.	FAF1320
C -----	FAF1330
C IF (INSTAT(L,J).EQ.0) GO TO 1200	FAF1340
IIINVR=1+7*(INVPH(L,J,1)-1)	FAF1350
CALL DDERIV (TREF)	FAF1360
DO 1100 K=1,7	FAF1370
DC(K+IIINVR-1)=DC(K+IIINVR-1)+DDDC(K)*SGN(2)*SC*DYDC(4)	FAF1380
1100 CONTINUE	FAF1390
1200 CONTINUE	FAF1400
C -----	FAF1410
C CALL DDERIV TO CALCULATE THE DERIVATIVE WITH RESPECT TO D FOR	FAF1420
C HIGH AND LOW TEMPERATURE PHASE AT TEMPERATURE OF	FAF1430
C INVERSION. PROCEED TO ADJUST DC ACCORDINGLY.	FAF1440
C -----	FAF1450
C LSTINV=IIINVR(L,J)	FAF1460
DO 1500 LL=1,LSTINV	FAF1470
CALL DDERIV (TINV(L,J,LL))	FAF1480
C -----	FAF1490
C	FAF1500
C	FAF1510
C -----	FAF1520
C IF (INVSC(L,J).EQ.0) GO TO 1300	FAF1530
IF (LL.NE.LSTINV) GO TO 1300	FAF1540
SGN(2)=SGN(2)/STCCEF(INVSC(L,J))	FAF1550
1300 CONTINUE	FAF1560
DO 1400 LLL=1,2	FAF1570
IIINVR=1+7*(INVPH(L,J,(LL+LLL-1))-1)	FAF1580
DO 1400 K=1,7	FAF1590
DC(K+IIINVR-1)=DC(K+IIINVR-1)+DDDC(K)*SGN(LLL)*SC*DYDC(4)	FAF1600
1400 CONTINUE	FAF1610
1500 CONTINUE	FAF1620
1600 CONTINUE	FAF1630
C -----	FAF1640
C COMPLETE THE CALCULATION OF DC BY ADDING THE DERIVATIVE AT T(OBS).	FAF1650
C	FAF1660
DO 1700 K=1,7	FAF1670
DC(K+INDEX-1)=DC(K+INDEX-1)+SC*DYDC(K)	FAF1680
1700 CONTINUE	FAF1690
1800 CONTINUE	FAF1700
C -----	FAF1710
C ALL DERIVATIVES HAVE BEEN CALCULATED. NOW CALCULATE YC BY	FAF1720
C SUMMING THE PRODUCT DC*P.	FAF1730
C -----	FAF1740
DO 1900 K=1,NP	FAF1750
YC=YC+P(K)*DC(K)	FAF1760
1900 CONTINUE	FAF1770
C -----	FAF1780
C RETURN	FAF1790
C -----	FAF1800
C RETURN	FAF1810
C -----	FAF1820

C	FORMAT STATEMENTS	EA1830
C	-----	EA1840
2000	FORMAT (6CHOIN EA1820 I IS GREATER THAN NC, THE NUMBER OF OBSERVATE	EA1850
	1IONS./64H THEREFORE, I (THE COMPUTER) AM QUITTING. THE PROBLEM IS	EA1860
	2YOURS.)	EA1870
2100	FORMAT (1F0.10A8/1H)	EA1880
	END	EA1890-

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C      SUBROUTINE YDERIV (T,J)
C      -----YCE 10
C      -----YCE 20
C      -----YCE 30
C      YDERIV
C      -----YCE 40
C      THIS VERSION WRITTEN 3/09/72 BY HAAS.
C      -----YCE 50
C      LAST REVISED 8/05/72 BY HAAS.
C      -----YCE 60
C      -----YCE 70
C      -----YCE 80
C      IMPLICIT REAL*8(A-H,C-Z)
C      -----YCE 90
C      DIMENSION DYCC(7),SCINV(2),DDCC(7),STCOEF(10)
C      -----YCE 100
C      -----YCE 110
C      COMMON BLOCKS
C      NAME ROUTINES
C      -----YCE 120
C      EARTH MAIN PROGRAM, CRGLS2, EAFW20, PLTOLT
C      -----YCE 130
C      AIR MAIN PROGRAM, CRGLS2, TEST2J, EAFW20
C      -----YCE 140
C      PUTOUT AND UNICL.
C      -----YCE 150
C      FIRE MAIN PROGRAM, CRGLS2, TEST2J, EAFW20
C      -----YCE 160
C      WATER MAIN PROGRAM, EAFW20, YDERIV, DDERIV,
C      -----YCE 170
C      PUTOUT, FN, DIF, AND PLOCK DATA.
C      -----YCE 180
C      TIME MAIN PROGRAM, PLTOUT
C      -----YCE 190
C      SPACE MAIN PROGRAM, EAFW20, YDERIV, DDERIV,
C      -----YCE 200
C      AND PLTOUT
C      -----YCE 210
C      MAN MAIN PROGRAM, PLTOUT
C      -----YCE 220
C      -----YCE 230
C      -----YCE 240
C      COMMON /WATER/ZERC, CNE, TWC, THREE, FOUR, SIX, R, F,
C      1 SCINV, TRIF, STCOEF,DIEC,A,B,THETA
C      -----YCE 250
C      COMMON /SPACE/ DDCC, DYCC, SC, TC
C      -----YCE 260
C      -----YCE 270
C      -----YCE 280
C      CALCULATE THE APPROPRIATE TEMPERATURE TERM IN THE DERIVATIVE
C      -----YCE 290
C      AND RETURN. --APPROPRIATE AS INDICATED BY J.
C      -----YCE 300
C      -----YCE 310
C      GO TO 1100,200,300,400,500,600,700,800,1000,1100,1200,1300,1400,1500, J
C      -----YCE 320
C      100 CONTINUE
C      -----YCE 330
C      -----YCE 340
C      -----YCE 350
C      THE DERIVATIVE FOR HEAT CAPACITY OF NON-IONIC SPECIES.
C      -----YCE 360
C      -----YCE 370
C      DYCC(1)=ONE
C      -----YCE 380
C      DYCC(2)=TWO*T
C      -----YCE 390
C      DYCC(3)=ONE/(T*T)
C      -----YCE 400
C      DYCC(4)=ZERO
C      -----YCE 410
C      DYCC(5)=ZERO
C      -----YCE 420
C      DYCC(6)=T*T
C      -----YCE 430
C      DYCC(7)=ONE/DSQRT(T)
C      -----YCE 440
C      RETURN
C      -----YCE 450
C      200 CONTINUE
C      -----YCE 460
C      -----YCE 470
C      THE DERIVATIVE FOR ENTROPY OF NON-IONIC SPECIES.
C      -----YCE 480
C      -----YCE 490
C      DYCC(1)=CLCG(T)
C      -----YCE 500
C      DYCC(2)=TWC*T
C      -----YCE 510
C      DYCC(3)=-CNE/ITWO*T*T)
C      -----YCE 520
C      DYCC(4)=ZERO
C      -----YCE 530
C      DYCC(5)=ONE
C      -----YCE 540
C      DYCC(6)=T*T/TWO
C      -----YCE 550
C      DYCC(7)=-TWO/DSQRT(T)
C      -----YCE 560
C      RETURN
C      -----YCE 570
C      300 CONTINUE
C      -----YCE 580
C      -----YCE 590
C      THE DERIVATIVE FOR THE ENTHALPY OF NON-IONIC SPECIES.
C      -----YCE 600

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C -----YCE 610
CYCC(1)=T-----YCE 620
CYCC(2)=T*T-----YCE 630
DYCC(3)=-CNE/T-----YCE 640
DYCC(4)=ONE-----YCE 650
CYCC(5)=ZERO-----YCE 660
CYCC(6)=(T**3)/THREE-----YCE 670
CYCC(7)=TWO*DSQRT(T)-----YCE 680
RETURN-----YCE 690
400 CONTINUE-----YCE 700
C -----YCE 710
C THE DERIVATIVE FOR THE GIBBS ENERGY OF NON-IONIC SPECIES.-----YCE 720
C -----YCE 730
CYCC(1)=T-T*CLGG(T)-----YCE 740
DYCC(2)=-1*T-----YCE 750
DYCC(3)=-CNE/(TWO*T)-----YCE 760
DYCC(4)=CNE-----YCE 770
CYCC(5)=-T-----YCE 780
DYCC(6)=-T**3/SIX-----YCE 790
DYCC(7)=FOUR*DSQRT(T)-----YCE 800
RETURN-----YCE 810
500 CONTINUE-----YCE 820
C -----YCE 830
C THE DERIVATIVE FOR THE EQUILIBRIUM CONSTANT OF ION-IONIC-----YCE 840
C SPECIES.-----YCE 850
C -----YCE 860
CYCC(1)=(CLGG(T)-CNE)/R-----YCE 870
CYCC(2)=T/R-----YCE 880
DYCC(3)=CAL/(TWO*R*T)-----YCE 890
DYCC(4)=-CNE/(R*T)-----YCE 900
CYCC(5)=CNE/R-----YCE 910
DYCC(6)=(T*T)/(SIX*R)-----YCE 920
DYCC(7)=-FOUR/(R*DSQRT(T))-----YCE 930
RETURN-----YCE 940
600 CONTINUE-----YCE 950
C -----YCE 960
C THE DERIVATIVE FOR THE CELL POTENTIAL FOR NON-IONIC SPECIES.-----YCE 970
C -----YCE 980
CYCC(1)=(T*CLGG(T)-T)/F-----YCE 990
DYCC(2)=(T*T)/F-----YCE1000
DYCC(3)=CNE/(TWO*F*T)-----YCE1010
DYCC(4)=-CNE/F-----YCE1020
CYCC(5)=T/F-----YCE1030
DYCC(6)=(T**3)/(SIX*F)-----YCE1040
DYCC(7)=-FOUR*DSQRT(T)/F-----YCE1050
RETURN-----YCE1060
700 CONTINUE-----YCE1070
C -----YCE1080
C THE DERIVATIVE FOR THE RELATIVE HEAT CONTENT OF NON-IONIC-----YCE1090
C SPECIES.-----YCE1100
C -----YCE1110
IF (SC.LT.0) GO TO 800-----YCE1120
CYCC(1)=T-----YCE1130
CYCC(2)=T*T-----YCE1140
DYCC(3)=-CNE/T-----YCE1150
DYCC(4)=ONE-----YCE1160
CYCC(5)=ZERO-----YCE1170
DYCC(6)=(T**3)/THREE-----YCE1180
DYCC(7)=TWO*DSQRT(T)-----YCE1190
RETURN-----YCE1200
800 CONTINUE-----YCE1210

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	DYCC(1)=TC	YDE1220
	DYCC(2)=TC*TC	YDE1230
	DYCC(3)=-CNE/TC	YDE1240
	DYCC(4)=CNE	YDE1250
	DYCC(5)=ZERO	YDE1260
	DYCC(6)=(TC**3)/THREE	YDE1270
	DYCC(7)=TWO*DSQRT(TO)	YDE1280
	RETURN	YDE1290
900	CONTINUE	YDE1300
C	-----	YDE1310
C	THE DERIVATIVE FOR THE HEAT CAPACITY OF IONIC SPECIES.	YDE1320
C	-----	YDE1330
	DYCC(1)=ONE	YDE1340
	DYCC(2)=TWO*T	YDE1350
	DYCC(3)=CNE/(T*T)	YDE1360
	DYCC(4)=ZERO	YDE1370
	DYCC(5)=ZERO	YDE1380
	DYCC(6)=T*T	YDE1390
	FNT=FN(T)	YDE1400
	DYCC(7)=-T*DI(T)*(A*FNT*A*FNT+A*FNT*A*A*FNT*TWO/THETA+ONE/(THETA	YDE1410
	1THETA))	YDE1420
	RETURN	YDE1430
1000	CONTINUE	YDE1440
C	-----	YDE1450
C	THE DERIVATIVE FOR THE ENTROPY OF IONIC SPECIES.	YDE1460
C	-----	YDE1470
	DYCC(1)=DLOG(T)	YDE1480
	DYCC(2)=TWO*T	YDE1490
	DYCC(3)=-CNE/(TWO*T*T)	YDE1500
	DYCC(4)=ZERO	YDE1510
	DYCC(5)=CNE	YDE1520
	DYCC(6)=T*T/TWO	YDE1530
	DYCC(7)=-DI(T)*(A*FN(T)+ONE/THETA)	YDE1540
	RETURN	YDE1550
1100	CONTINUE	YDE1560
C	-----	YDE1570
C	THE DERIVATIVE FOR THE ENTHALPY OF IONIC SPECIES.	YDE1580
C	-----	YDE1590
	DYCC(1)=T	YDE1600
	DYCC(2)=T*T	YDE1610
	DYCC(3)=-CNE/T	YDE1620
	DYCC(4)=CNE	YDE1630
	DYCC(5)=ZERO	YDE1640
	DYCC(6)=(T**3)/THREE	YDE1650
	DYCC(7)=DI(T)*(CNE-A*T*FN(T)-T/THETA)	YDE1660
	RETURN	YDE1670
1200	CONTINUE	YDE1680
C	-----	YDE1690
C	THE DERIVATIVE FOR THE GIBBS ENERGY OF IONIC SPECIES.	YDE1700
C	-----	YDE1710
	DYCC(1)=T-T*DLOG(T)	YDE1720
	DYCC(2)=-T*T	YDE1730
	DYCC(3)=-CNE/(TWO*T)	YDE1740
	DYCC(4)=CNE	YDE1750
	DYCC(5)=-T	YDE1760
	DYCC(6)=-T**3/SIX	YDE1770
	DYCC(7)=DI(T)	YDE1780
	RETURN	YDE1790
1300	CONTINUE	YDE1800
C	-----	YDE1810
C	THE DERIVATIVE FOR THE EQUILIBRIUM CONSTANT OF IONIC	YDE1820

C	SPECIES.	YCE1830
C	-----	YCE1840
	DYCC(1)=(CLOG(T)-CNE)/R	YCE1850
	CYCC(2)=T/P	YCE1860
	DYCC(3)=CNE/(TWC*F*T+T)	YCE1870
	DYCC(4)=-CNE/(R*T)	YCE1880
	DYCC(5)=CNE/R	YCE1890
	DYCC(6)=(T+T)/(SIX*R)	YCE1900
	DYCC(7)=-CIE(T)/(R*T)	YCE1910
	RETURN	YCE1920
1400	CONTINUE	YCE1930
C	-----	YCE1940
C	THE DERIVATIVE FOR THE CELL POTENTIAL OF IGNIC SPECIES.	YCE1950
C	-----	YCE1960
	DYCC(1)=(T*CLOG(T)-T)/F	YCE1970
	DYCC(2)=(T+T)/F	YCE1980
	DYCC(3)=CNE/(TWC*F*T)	YCE1990
	DYCC(4)=-CNE/F	YCE2000
	DYCC(5)=T/F	YCE2010
	DYCC(6)=(T**3)/(SIX*F)	YCE2020
	DYCC(7)=-CIE(T)/F	YCE2030
	RETURN	YCE2040
1500	CONTINUE	YCE2050
C	-----	YCE2060
C	THE DERIVATIVE FOR THE RELATIVE HEAT CONTENT OF IGNIC	YCE2070
C	SPECIES.	YCE2080
C	-----	YCE2090
	IF (SC.LT.0) GO TO 1600	YCE2100
	DYCC(1)=T	YCE2110
	DYCC(2)=T+T	YCE2120
	DYCC(3)=-CNE/T	YCE2130
	DYCC(4)=CNE	YCE2140
	DYCC(5)=ZERO	YCE2150
	DYCC(6)=(T**3)/THREE	YCE2160
	DYCC(7)=DIE(T)*(CNE-A*T*FN(T)-T/THETA)	YCE2170
	RETURN	YCE2180
1600	CONTINUE	YCE2190
	DYCC(1)=TC	YCE2200
	DYCC(2)=TC*TO	YCE2210
	DYCC(3)=-CNE/TC	YCE2220
	DYCC(4)=CNE	YCE2230
	DYCC(5)=ZERO	YCE2240
	DYCC(6)=(TC**3)/THREE	YCE2250
	DYCC(7)=CIE(TO)*(CNE-A*TO*FN(TO)-TO/THETA)	YCE2260
	RETURN	YCE2270
C	-----	YCE2280
	END	YCE2290-

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C SUBROUTINE CDERIV (T) CCE 10
C ----- CCE 20
C CCE 30
C CCE 40
C CCE 50
C CCE 60
C THIS VERSION WAS WRITTEN 3/09/72 BY HAAS. CCE 70
C LAST REVISED 8/05/72 BY HAAS. CCE 80
C ----- CCE 90
C IMPLICIT REAL*8(A-H,O-Z) CCE 100
C DIMENSION DCCC(7),SCINV(2),DYCC(7) CCE 110
C ----- CCE 120
C COMMON BLOCKS CCE 130
C NAME ROUTINES CCE 140
C EARTH MAIN PROGRAM, CRGLS2, EAFW20, PLTOUT CCE 150
C AIR MAIN PROGRAM, CRGLS2, TEST2J, EAFW20 CCE 160
C PUTOUT AND UNIQUE. CCE 170
C FIRE MAIN PROGRAM, CRGLS2, TEST2J, EAFW20 CCE 180
C WATER MAIN PROGRAM, EAFW20, YCERIV, CDERIV, CCE 190
C PUTOUT, FN, CIE, AND PLOCK DATA. CCE 200
C TIME MAIN PROGRAM, PLTOUT CCE 210
C SPACE MAIN PROGRAM, EAFW20, YCERIV, CDERIV, CCE 220
C AND PUTPLT CCE 230
C MAN MAIN PROGRAM, PLTOUT CCE 240
C ----- CCE 250
C COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, F, CCE 260
C SCINV, TREF, STOFF, DIED, A, B, THETA CCE 270
C COMMON /SPACE/ DCCC, DYCC, SC, TO CCE 280
C ----- CCE 290
C CALCULATE THE DERIVATIVE OF -G- WITH RESPECT TO THE OTHER CCE 300
C CONSTANTS WHERE THE GIBBS ENERGY IS 0.0 AS IS THE CCE 310
C CASE FOR ELEMENTS AT 298.15 KELVIN OR AT THE TEMPERATURE OF CCE 320
C INVERSION. CCE 330
C ----- CCE 340
C DCCC(1)=T*DLGG(1)-T CCE 350
C DCCC(2)=T*T CCE 360
C DCCC(3)=ONE/(TWO*T) CCE 370
C DCCC(4)=-ONE CCE 380
C DCCC(5)=T CCE 390
C DCCC(6)=(T**3)/SIX CCE 400
C DCCC(7)=-FCUR*DSOPT(T) CCE 410
C RETURN CCE 420
C END

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	DOUBLE PRECISION FUNCTION DIE(T)	CIE	10
	IMPLICIT REAL*8(A-H,C-Z)	CIE	20
	DIMENSION STCOEF(10),SCINV12)	CIE	30
C	-----	CIE	40
C	COMMON BLOCKS	CIE	50
C	NAME ROUTINES	CIE	60
C	EARTH MAIN PROGRAM, DRCLS2, EAFW20, PUTOUT	CIE	70
C	AIR MAIN PROGRAM, DRCLS2, TEST20, EAFW20	CIE	80
C	PUTOUT AND UNICL.	CIE	90
C	FIRE MAIN PROGRAM, CPCLS2, TEST20, EAFW20	CIE	100
C	WATER MAIN PROGRAM, EAFW20, YDERIV, DDERIV,	CIE	110
C	PUTOUT, FV, DIS, AND PLOCK DATA.	CIE	120
C	TIME MAIN PROGRAM, PUTJLT	CIE	130
C	SPACE MAIN PROGRAM, EAFW20, YDERIV, DDERIV,	CIE	140
C	AND PUTOUT	CIE	150
C	MAN MAIN PROGRAM, PUTOUT	CIE	160
C	-----	CIE	170
	COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, F,	CIE	180
	1 SCINV, TRIF, STCOEF, DIERO, A, B, THETA	CIE	190
	DIE=CSXPI(FN(T))*T/THETA)/DIERO	CIE	200
	RETURN	CIE	210
	END	CIE	220-

	DOUBLE PRECISION FUNCTION FN(T)	FN	10
	IMPLICIT REAL*8(A-H,C-Z)	FN	20
	DIMENSION STCOEF(10),SCINVI(2)	FN	30
C	-----	FN	40
C	COMMON BLOCKS	FN	50
C	NAME ROUTINES	FN	60
C	EARTH MAIN PROGRAM, ORCLS2, EAFW20, PUTOUT	FN	70
C	AIR MAIN PROGRAM, ORCLS2, TEST20, EAFW20	FN	80
C	PUTOUT AND UNICL.	FN	90
C	FIRE MAIN PROGRAM, ORCLS2, TEST20, EAFW20	FN	100
C	WATER MAIN PROGRAM, EAFW20, YDERIV, CDERIV,	FN	110
C	PUTOUT, FN, CIE, AND PLOCK DATA.	FN	120
C	TIME MAIN PROGRAM, PLTCUT	FN	130
C	SPACE MAIN PROGRAM, EAFW20, YDERIV, CDERIV,	FN	140
C	AND PUTOUT	FN	150
C	MAN MAIN PROGRAM, PLTCUT	FN	160
C	-----	FN	170
	COMMON /WATER/ZERO, ONE, TWO, THREE, FOUR, SIX, R, P,	FN	180
	1 SCINV, TRSF, STCOEF, CIEO, A, B, THETA	FN	190
	FN=DEXP(B*A*T)	FN	200
	RETURN	FN	210
	END	FN	220-

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C      SUBROUTINE UNIQUE (YC,I,J,JCFLAG)
C      -----
C      CUMMY SUBROUTINE UNIQUE -- RETURNS ERROR STATEMENT IF CALLED.
C      -----
C      UNIQUE IS TO BE PROGRAMMED BY THE USER. UNIQUE IS INTENDED
C      TO SUPPLY YC AND CC(KI(NP),NE,0) FOR THOSE DATA SETS NOT
C      COVERED BY THE ROUTINES EAFW20, YCERIV, AND ODERIV.
C      -----
C      THE SUBROUTINE UNIQUE WILL BE CALLED WHEN THE INDEX IGO(I) IS
C      GREATER THAN 7.
C      -----
C      ARGUMENTS--
C      YC -- YCALC RETURNED BY UNIQUE FROM CURRENT VALUES OF
C      THE PARAMETERS P(I).
C      I -- INDEX FOR THE I-TH OBSERVATION.
C      J -- INDEX FOR THE J-TH DATA SET.
C      JCFLAG -- IF UNIQUE IS CALLED AT REGRESSION TIME,
C      JCFLAG IS ZERO AND THE DERIVATIVES
C      CC(I) MUST BE RETURNED.
C      IF UNIQUE IS CALLED AT PLOT TIME, JCFLAG
C      IS NOT ZERO AND THE DERIVATIVES NEED
C      NOT BE RETURNED.
C      -----
C      IMPLICIT REAL*8(A-H,C-Z)
C      DIMENSION COEF(6,70),PNAME(20),TINV(6,70,4),IPHASE(5,70),
C      1 NPHASE(70),IKOUNT(70),IGC(70),ISTATE(6,70),NINVER(6,70),
C      2 INSTAT(6,70),INVPH(6,70,5),INVSC(6,70)
C      -----
C      COMMON BLOCKS
C      NAME          ROUTINES
C      EARTH         MAIN PROGRAM, CRCLS2, EAFW20, PUTOUT
C      AIR           MAIN PROGRAM, CRCLS2, TEST20, EAFW20
C      FIRE          MAIN PROGRAM, CRCLS2, TEST20, EAFW20
C      WATER         MAIN PROGRAM, EAFW20, YCERIV, ODERIV,
C      TIME          MAIN PROGRAM, PLTCUT
C      SPACE         MAIN PROGRAM, EAFW20, YCERIV, ODERIV,
C      MAN           AND PUTOUT
C      MAIN          MAIN PROGRAM, PLTCUT
C      -----
C      COMMON /EARTH/ COEF,PNAME,TINV,IPHASE,NPHASE,IKOUNT,IGC,NSETS,
C      1 ISTATE,NINVER,INSTAT,INVPH,INVSC,LISTP
C      WRITE (6,100) J,J,IGC(J)
C      STOP
C      100 FORMAT (6F30.9,13,35H-TH DATA SET CALLED UNIQUE FROM EAFW20./5H
C      1IGC(12,17H) HAS A VALUE OF ,16,35H BUT UNIQUE IS CURRENTLY UNPROGRAMMED
C      2RAM460.)
C      END
C      -----
C      UNI 10
C      UNI 20
C      UNI 30
C      UNI 40
C      UNI 50
C      UNI 60
C      UNI 70
C      UNI 80
C      UNI 90
C      UNI 100
C      UNI 110
C      UNI 120
C      UNI 130
C      UNI 140
C      UNI 150
C      UNI 160
C      UNI 170
C      UNI 180
C      UNI 190
C      UNI 200
C      UNI 210
C      UNI 220
C      UNI 230
C      UNI 240
C      UNI 250
C      UNI 260
C      UNI 270
C      UNI 280
C      UNI 290
C      UNI 300
C      UNI 310
C      UNI 320
C      UNI 330
C      UNI 340
C      UNI 350
C      UNI 360
C      UNI 370
C      UNI 380
C      UNI 390
C      UNI 400
C      UNI 410
C      UNI 420
C      UNI 430
C      UNI 440
C      UNI 450
C      UNI 460
C      UNI 470
C      UNI 480
C      UNI 490-

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SUBROUTINE PLTCUT (J)                                PUT 10
IMPLICIT REAL*8(A-H,C-Z)                             PUT 20
LOGICAL*1 BCC,LABEL                                PUT 30
REAL*4 TITLE,ACOFF                                PUT 40
DIMENSION SGN(2),A(7,7)                            PUT 50
DIMENSION COEF(6,7),PNAME(20),TINV(6,70,4),IPHA(6,70), PUT 60
1  NPHASE(70),TKJLNT(70),IGC(70),ISTATE(6,70),NINVER(6,70), PUT 70
2  ISTAT(6,70),INVPH(6,70,5),INVSC(6,70)            PUT 80
DIMENSION X(2,1200),YC(1200),SIGYC(1200),P(140),KI(140), PUT 90
1  DC(140),PD(140),TITLE(20)                        PUT 100
DIMENSION SCINV(2),STCOEF(10),YLSNO(2),TK(19,2),TYPE(14),NSCALE(5) PUT 110
1  ,LABEL(50)                                         PUT 120
DIMENSION DDEC(7),DYDC(7)                            PUT 130
DIMENSION AA (140)                                    PUT 140
-----PUT 150
C      COMMON BLOCKS                                PUT 160
C      NAME      ROUTINES                            PUT 170
C      EARTH      MAIN PROGRAM, DRGLS2, EAFW20, PUTOUT PUT 180
C      AIR         MAIN PROGRAM, DRGLS2, TEST20, EAFW20 PUT 190
C                   PUTOUT AND UNISLE.                PUT 200
C      FIRE        MAIN PROGRAM, DRGLS2, TEST20, EAFW20 PUT 210
C      WATER       MAIN PROGRAM, EAFW20, YDERIV, DDERIV, PUT 220
C                   PUTOUT, FN, DIE, AND PLCKC DATA. PUT 230
C      TIME        MAIN PROGRAM, PLTCUT                PUT 240
C      SPACE       MAIN PROGRAM, EAFW20, YDERIV, DDERIV, PUT 250
C                   AND PLTPT                            PUT 260
C      MAN         MAIN PROGRAM, PLTCUT                PUT 270
C-----PUT 280
COMMON /EARTH/ COEF,PNAME,TINV,IPHA,NPHASE,IKCNT,IGC,NSETS, PUT 290
1  ISTATE,NINVER,ISTAT,INVPH,INVSC,LISTP            PUT 300
COMMON /AIR/ X, P, DC, TITLE, YC, SIGYC, PD, KI, AC, NV, NX, IW, PUT 310
1  NP, NO, ISING, ISTOP, IL, JOFLAG                PUT 320
COMMON /WATER/ZERC, ONE, TWO, THREE, FOUR, SIX, F, F, PUT 330
1  SCINV, TREF, STCOEF, DIEO, ADIS, ECIE, THETA, YESNO, TK, PUT 340
2  ASTAR, TYPE, NL, NSCALE, LABEL, BCC              PUT 350
COMMON /TIME/ DATE                                PUT 360
COMMON /SPACE/ DDEC, DYDC, SC, TO                  PUT 370
COMMON /MAN/ AA                                    PUT 380
CPRIME=ZERC                                         PUT 390
LSTPHA=NPHASE(J)                                    PUT 400
DO 1200 L=1,LSTPHA                                  PUT 410
INDEX=1/(IPHA(L,J)-1)                               PUT 420
D=C.00J                                              PUT 430
IF (ISTATE(L,J).NE.1) GO TO 200                      PUT 440
CALL DDERIV (TREF)                                   PUT 450
DO 100 K=1,7                                         PUT 460
D=D+P(INDEX*K-1)*DDEC(K)                            PUT 470
100 CONTINUE                                         PUT 480
GO TO 900                                           PUT 490
200 CONTINUE                                         PUT 500
IF (NINVER(L,J).EQ.0) GO TO 900                    PUT 510
DO 300 I=1,2                                         PUT 520
SGN(I)=SCINV(I)                                       PUT 530
300 CONTINUE                                         PUT 540
IF (INVSC(L,J).EQ.0) GO TO 500                      PUT 550
DO 400 LLL=1,2                                       PUT 560
SGN(LLL)=SGN(LLL)*STCOEF(INVSC(L,J))                PUT 570
400 CONTINUE                                         PUT 580
500 CONTINUE                                         PUT 590
IF (ISTAT(L,J).EQ.0) GO TO 700                      PUT 600

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INDEX2=I+7*(INVPH(L,J,1)-1)	PLT 610
CALL DDERIV (TREF)	PLT 620
DO 600 K=1,7	PUT 630
C=C+P(INDEX2+K-1)*CCCC(K)*SGN(2)	PUT 640
600 CONTINUE	PLT 650
700 CONTINUE	PLT 660
LSTINV=NINVER(L,J)	PUT 670
DO 800 LST=1,LSTINV	PLT 680
IF ((LST.EQ.LSTINV).AND.(INVSC(L,J).NE.0)) SGN(2)=SGN(2)/STCOEF(INVSC(L,J))	PLT 690
CALL DDERIV (TINV(L,J,LST))	PLT 700
DO 800 LLL=1,2	PLT 710
INDEX2=I+7*(INVPH(L,J,LST+LLL-1)-1)	PUT 720
DO 800 K=1,7	PLT 730
C=C+P(INDEX2+K-1)*CCCC(K)*SGN(LLL)	PUT 740
800 CONTINUE	PLT 750
900 CONTINUE	PUT 760
DO 1000 K=1,7	PUT 770
A(L,K)=P(INDEX+K-1)	PUT 780
1000 CONTINUE	PLT 790
A(L,4)=A(L,4)+D	PUT 800
DO 1100 K=1,7	PUT 810
AA(INDEX+K-1)=A(L,K)	PUT 820
1100 CONTINUE	PUT 830
1200 CONTINUE	PLT 840
LST=LSTPH+1	PUT 850
DO 1300 K=1,7	PUT 860
A(LST,K)=C.000	PLT 870
1300 CONTINUE	PUT 880
DO 1500 L=1,LSTPHA	PUT 890
DO 1500 K=1,7	PUT 900
IF ((K.EQ.7).AND.(ISTATE(L,J).EQ.-1)) GO TO 1400	PUT 910
A(LST,K)=A(LST,K)+A(L,K)*COEF(L,J)	PUT 920
GO TO 1500	PLT 930
1400 CPRIME=CPRIME+A(L,K)*COEF(L,J)	PLT 940
1500 CONTINUE	PLT 950
WRITE (6,1900) DATE	PUT 960
DO 1600 L=1,LSTPHA	PUT 970
ACCOEF=COEF(L,J)	PLT 980
WRITE (6,2000) PNAME(IPHASE(L,J)),ACCOEF,(A(L,K),K=1,7)	PUT 990
1600 CONTINUE	PUT1000
IF ((IPHASE(J).EQ.1).CR.(JGO(J).GE.7)) GO TO 1800	PLT1010
IF (CPRIME.EQ.ZERO) GO TO 1700	PLT1020
WRITE (6,2200)	PLT1030
WRITE (6,2300) (A(LST,K),K=1,7),CPRIME	PUT1040
GO TO 1800	PLT1050
1700 CONTINUE	PUT1060
WRITE (6,2100)	PLT1070
WRITE (6,2300) (A(LST,K),K=1,7)	PUT1080
1800 CONTINUE	PLT1090
RETURN	PUT1100
1900 FORMAT (1F0/1H0,A8,1CH-----/6HOPHASE,8X,4HCOEF,9X,7H'A'/'G',1P	PUT1110
13X,3H'B',15X,3H'C',15X,3H'D',15X,3H'E',15X,3H'F')	PLT1120
2000 FORMAT (1F0,A8,4X,F6.3,1X,1P6018.7/1H ,15X,1P18.7)	PUT1130
2100 FORMAT (1F0/1H0,26X,7H'A'/'G',13X,3H'B',15X,3H'C',15X,3H'D',15X,3H'E',15X,3H'F')	PLT1140
1'F',15X,3H'F')	PUT1150
2200 FORMAT (1F0/1H0,26X,7H'A'/'G',9X,12H'B'/'G(IQN)',10X,3H'C',15X,3H'D',15X,3H'E',15X,3H'F')	PLT1160
10',15X,3H'E',15X,3H'F')	PUT1170
2300 FORMAT (20HOREACTION CONSTANTS ,1P6018.7/(1F ,15X,1P2018.7))	PLT1180
END	PUT1190
	PUT1200-

SUBROUTINE PRPLOT	
IMPLICIT LOGICAL*1(W), LOGICAL*1(K)	PRP 10
DIMENSION NSCALE(5), ABNOS(26), X(1), Y(1)	PRP 20
LOGICAL*1 NOS(10)/'0','1','2','3','4','5','6','7','8','9'/	PRP 30
LOGICAL*1 IMAGE(5000), CF, LABEL(50)	PRP 40
LOGICAL*1 VC, HC, FC(1(19), FOR2(15), FOR3(19), AC, BL, HF, HF1	PRP 50
REAL*8 FCX(1(3), FCX2(2), FCX3(3))	PRP 60
INTEGER*2 VCR	PRP 70
EQUIVALENCE(FOR1, FCX1), (FOR2, FCX2), (FOR3, FCX3), (VC, VCR)	PRP 80
DATA HC/'-','/','NC','+',',','BL',' ','HF','F','HF1','.'/	PRP 90
DATA FCX1/'(1XA1,F5','2, 121','A1) '	PRP 100
DATA FCX2/'(1XA1, 9','X121A1) '	PRP 110
DATA FCX3/'(1HOF .',' , F .',.) '	PRP 120
DATA VCR/24F00/	PRP 130
DATA KPLCT1/.FALSE./, KPLCT2/.FALSE./	PRP 140
DATA KABSC, KORD, KPGTGL/3*.FALSE./	PRP 150
	PRP 160
ENTRY PLOT1(NSCALF, NFL, NSBH, NVL, NSBV)	PRP 170
KPLCT1=.TRUE.	PRP 180
KPLCT2=.FALSE.	PRP 190
NH=IABS(NFL)	PRP 200
NSF=IABS(NSBH)	PRP 210
NV=IABS(NVL)	PRP 220
NSV=IABS(NSBV)	PRP 230
NSCL=NSCALF(1)	PRP 240
IF (NH*NSF*NV*NSV.NE.0) GO TO 200	PRP 250
WRITE (6,100)	PRP 260
100 FORMAT (T5,'SOME PLOT1 ARG. ILLEGALLY 0')	PRP 270
KPLCT=.FALSE.	PRP 280
RETURN	PRP 290
200 KPLCT=.TRUE.	PRP 300
IF (NV.LE.25) GO TO 400	PRP 310
WRITE (6,300)	PRP 320
KPLCT=.FALSE.	PRP 330
300 FORMAT (T5,'NO. OF VERTICAL LINES >25')	PRP 340
RETURN	PRP 350
400 CONTINUE	PRP 360
NV=NV-1	PRP 370
NVP=NVP+1	PRP 380
NDH=NH*NSF	PRP 390
NDHP=NDH+1	PRP 400
NDV=NV*NSV	PRP 410
NDVP=NDV+1	PRP 420
NIG=(NDHP*NDVP)	PRP 430
IF (NDV.LE.120) GO TO 600	PRP 440
KPLCT=.FALSE.	PRP 450
WRITE (6,500)	PRP 460
500 FORMAT (T5,'WIDTH OF GRAPH >121')	PRP 470
PETURN	PRP 480
600 CONTINUE	PRP 490
IF (NSCL.EQ.0) GO TO 700	PRP 500
FSY=10.**NSCALE(2)	PRP 510
FSX=10.**NSCALE(4)	PRP 520
IY=MINJ(IABS(NSCALE(3)),7)+1	PRP 530
IX=MINJ(IABS(NSCALE(5)),9)+1	PRP 540
GO TO 800	PRP 550
700 FSY=1.	PRP 560
FSX=1.	PRP 570
IY=4	PRP 580
IX=4	PRP 590
	PRP 600

800 FOR1(10)=ACS(1V)	PRP 610
NA=MINJ(I),NSV)-1	PRP 620
NS=NA-MING(N4,120-NOV)	PRP 630
NB=11-NS+NA	PRP 640
I1=NE/10	PRP 650
I2=NP-I1*10	PRP 660
FOR3(6)=ACS(I1+1)	PRP 670
FOR3(7)=ACS(I2+1)	PRP 680
FOR3(9)=ACS(NA+1)	PRP 690
IF (NV.GT.0) GO TC 1000	PRP 700
DO 900 J=11,18	PRP 710
900 FOR3(J)=EL	PRP 720
GO TC 1100	PRP 730
1000 I1=NV/10	PRP 740
I2=IV-I1*10	PRP 750
FOR3(11)=ACS(I1+1)	PRP 760
FOR3(12)=ACS(I2+1)	PRP 770
FOR3(13)=HF	PRP 780
I1=NSV/100	PRP 790
I3=ISV-I1*100	PRP 800
I2=I3/10	PRP 810
I3=I3-I2*10	PRP 820
FOR3(14)=ACS(I1+1)	PRP 830
FOR3(15)=ACS(I2+1)	PRP 840
FOR3(16)=ACS(I3+1)	PRP 850
FOR3(17)=HF1	PRP 860
FOR3(18)=FCF3(9)	PRP 870
1100 IF (KPLJT1) RETURN	PRP 880
KPLJT1=.TRUE.	PRP 890
C	PRP 900
ENTRY PLCT2(IMAGE,XMAX,XMIN,YMAX,YMIN)	PRP 910
KPLCT2=.TRUE.	PRP 920
IF (KPLCT1) GO TC 1200	PRP 930
NSCL=J	PRP 940
NH=5	PRP 950
NSH=10	PRP 960
NV=10	PRP 970
NSV=10	PRP 980
GO TC 200	PRP 990
1200 CONTINUE	PRP1000
IF (.NOT.KPLCT) RETURN	PRP1010
YMX=YMAX	PRP1020
DM=(YMAX-YMIN)/FLCAT(NDH)	PRP1030
CV=(XMAX-XMIN)/FLCAT(NCV)	PRP1040
DO 1300 I=1,NVP	PRP1050
1300 ABWDS(I)=(XMIN+FLCAT((I-1)*NSV)*CV)*FSX	PRP1060
DO 1400 I=1,NIMG	PRP1070
1400 IMAGE(I)=EL	PRP1080
DO 1800 I=1,NOHP	PRP1090
I2=I*NOVP	PRP1100
I1=I2-NOV	PRP1110
KNHOR=MOD(I-1,NSH).NE.0	PRP1120
IF (KNHOR) GO TO 1600	PRP1130
DO 1500 J=11,12	PRP1140
1500 IMAGE(J)=FC	PRP1150
1600 CONTINUE	PRP1160
DO 1800 J=11,12,NSV	PRP1170
IF (KNHOR) GO TO 1700	PRP1180
IMAGE(J)=AC	PRP1190
GO TO 1800	PRP1200
1700 IMAGE(J)=VC	PRP1210

1800	CONTINUE	PPP1220
	XMIN1=XMIN-DV/2.	PRP1230
	YMIN1=YMIN-DH/2.	PRP1240
	RETURN	PRP1250
C		PRP1260
	ENTRY PLCT3(CH,X,Y,N3)	PRP1270
	IF (KPLCT2) GO TC 2100	PRP1280
1900	WRITE (6,2000)	PRP1290
2000	FORMAT (TS,'PLCT2 MLST BE CALLED')	PRP1300
2100	CONTINUE	PRP1310
	IF (.NOT.KPLCT) RETURN	PRP1320
	IF (N3.GT.0) GO TC 2300	PRP1330
	KPLCT=.FALSE.	PRP1340
	WRITE (6,2200)	PRP1350
2200	FORMAT (TS,'PLOT3, APG2) 0')	PRP1360
	RETURN	PRP1370
2300	DO 3000 I=1,N3	PRP1380
	IF (CV) 2500,2400,2500	PRP1390
2400	CUM1=0	PRP1400
	GO TO 2600	PRP1410
2500	CONTINUE	PRP1420
	CUM1=(X(I)-XMIN1)/DV	PRP1430
2600	IF (CH) 2800,2700,2800	PRP1440
2700	CUM2=0	PRP1450
	GO TC 2900	PRP1460
2800	CONTINUE	PRP1470
	CUM2=(Y(I)-YMIN1)/DH	PRP1480
2900	CONTINUE	PRP1490
	IF (CUM1.LT.0..OR.CUM2.LT.0.) GO TO 3000	PRP1500
	IF (CUM1.GE.NDVP..CP.CUM2.GE.NDHP) GO TC 3000	PRP1510
	NX=1+INT(CUM1)	PRP1520
	NY=1+INT(CUM2)	PRP1530
	J=(NCHP-NY)*NDVP+NX	PRP1540
	IMAGE(J)=CH	PRP1550
3000	CONTINUE	PRP1560
	RETURN	PRP1570
C		PRP1580
	ENTRY PLCT4(NL,LABEL)	PRP1590
	ENTRY FPLCT4(NL,LABEL)	PRP1600
	IF (.NOT.KPLCT) RETURN	PRP1610
	IF (.NOT.KPLCT2) GO TC 1900	PRP1620
	DO 3200 I=1,NDHP	PRP1630
	IF (I.EQ.NDHP.ANC.KRECTGL) GO TO 3200	PRP1640
	WL=BL	PRP1650
	IF (I.LE.NL) WL=LABEL(I)	PRP1660
	I2=I*NDVP	PRP1670
	I1=I2-NDV	PRP1680
	IF (MOD(I-1,NSH).EQ.C.AND..NOT.KCRD) GO TC 3100	PRP1690
	WRITE (6,FCR2) WL,(IMAGE(J),J=I1,I2)	PRP1700
	GO TC 3200	PRP1710
3100	CONTINUE	PRP1720
	CRDNC=(YMX-FLOAT(I-1)*DH)*FSY	PRP1730
	IF (I.EQ.NDHP) CRDNC=YMIN	PRP1740
	WRITE (6,FCR1) WL,CRDNC,(IMAGE(J),J=I1,I2)	PRP1750
3200	CONTINUE	PRP1760
	IF (KABSC) GO TC 3300	PRP1770
	WRITE (6,FCR3) (ABNCS(J),J=1,NVP)	PRP1780
3300	RETURN	PRP1790
C		PRP1800
	ENTRY JMIT(LSW)	PRP1810
	KAPSC=MOD(LSW,2).EQ.1	PRP1820

KCRD=MJD(LSW,4).GE.2
K8CTGL=LSW.GE.4
PETUPN
END

PRP1830
PRP1840
PRP1850
PRP1860-