1620 GENERAL PROGRAM LIBRARY

Computation of Equilibrium Composition and Temperature of Chemical Reactions

9.3.018

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(fill out in typewriter, ink or pencil)

Program No.________________ Date________________

Program Name:____

1. Does the abstract adequately describe what the program is and what it does? Yes____ No____
   Comment____

2. Does the program do what the abstract says? Yes____ No____
   Comment____

3. Is the description clear, understandable, and adequate? Yes____ No____
   Comment____

4. Are the Operating Instructions understandable and in sufficient detail? Yes____ No____
   Comment____
   Are the Sense Switch options adequately described (if applicable)? Yes____ No____
   Are the mnemonic labels identified or sufficiently understandable? Yes____ No____
   Comment____

5. Does the source program compile satisfactorily (if applicable)? Yes____ No____
   Comment____

6. Does the object program run satisfactorily? Yes____ No____
   Comment____

7. Number of test cases run_____. Are any restrictions as to data, size, range, etc. covered adequately in description? Yes____ No____
   Comment____

8. Does the Program meet the minimal standards of COMMON? Yes____ No____
   Comment____

9. Were all necessary parts of the program received? Yes____ No____
   Comment____

10. Please list on the back any suggestions to improve the usefulness of the program. These will be passed onto the author for his consideration.

<u>Please return to:</u>

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11/1/65

Computation of Equilibrium Composition

and Temperature of Chemical Reactions

By

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and

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1620 Users Group No. 1235

March 9, 1966

Modifications or revisions to this program, as they occur, will be announced in the appropriate Catalog of Programs for IBM Data Processing Systems. When such an announcement occurs, users should order a complete new program from the Program Information Department.

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PROGRAM ABSTRACT

1. TITLE (If subroutine, state in Title): Computation of Equilibrium Composition and Temperature of Chemical Reactions
2. Author; Organization: Mae E. Meads, George E. McGowan - Baltimore Gas and Electric Company, Subject Classification:
   Date: 1 November, 1965 Users Group Membership Code: 1235
3. Direct Inquiries to Name: Engineering Computer Applications Group, Baltimore Gas and Electric Company, Baltimore, Maryland 21203 Phone: 539-8000
4. Description/Purpose: (5. Method; 6. Restriction/Range; When Applicable) Computes the equilibrium conditions for the combustion of any hydrocarbon in air or in any oxygen-nitrogen mixture of a given ratio. Uses method devised by Huff, Gordon and Morrell (1) involving solution of equations simultaneously by successive iterations. Restricted to adiabatic combustion processes in which the total number of elements and compounds does not exceed 7 and 13, respectively. Thermodynamic Functions Program is restricted to use with the Table of Coefficients included with the writeup.
7. Specifications (Check or fill in appropriate spaces):
   a. Storage used by program: 20K
   b. Equipment required by program:
      Card System X ; Magnetic Tape System ___; No. of Tapes ___;
      Paper Tape System ___; Disk File System ___; No. of Packs ___;
      TNS, TNF, MF ___; Auto divide ___; Indirect addressing ___;Floating point hardware ___;
      Other (specify) ___
      Can program be used on lesser Machine? No . Specify which requirements can be easily removed None
   c. Programming type (Check appropriate spaces):
      Fortran without Format ___; Fortran with Format ___;
      PDQ FORTRAN with Format X ;
      Fortran II ___;/Mainline, Complete X ; Subroutine or function subprogram(S or F) ___;
      Is the program a library (ie, SPS) function to the Fortran system checked? No ;
      SPS ___; SPS - 1620/1710 ___;
      Mainline, Complete ___; Macro ___; Subroutine ___;
      Other programming language: ___; Give details ___
   d. Language used in the writeup: English
8. Additional Remarks: The program consists of three parts referred to in the writeup as Thermodynamic Functions Program, Combustion Process I and Combustion Process II.

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* - First two (2) cards which zeroes core have been removed.

Deck 11 — Sample Problem No. 2 (Input)

Deck 12 — Control Card for Sample Problem No. 2 (One-Card-Input Data for Combustion Process II)

Deck 13 — Thermodynamic Coefficients for Temperature Range of 1500°-2500° for the Following Species: H_2, H_2O, OH, CO_2, CO, N_2, NO, O_2, H_2S, S_2, SO_2, SO_3, H, C, N, AR, O, S Used for Sample Problem No. 2

PROGRAM DESCRIPTIONS

COMPUTATION OF EQUILIBRIUM COMPOSITION AND TEMPERATURE OF CHEMICAL REACTIONS

GENERAL DESCRIPTION

The 1620 Program computes the equilibrium conditions for the combustion of any hydrocarbon in air or in any oxygen-nitrogen mixture of a given ratio. The final solution is expressed in terms of the partial pressures of each of the reaction products, "P_i", the equilibrium temperature "T", and the number of formula weights of the reactants, "A", which are involved in the chemical reaction.

A rapidly convergent approximation process that simultaneously determines both composition and temperature resulting from a chemical reaction is the method used in the program. This method was developed by the NACA Lewis Laboratory during 1948 and is applicable to a wide variety of problems.

The program, written for the 1620 computer in FORTRAN language, consists of three passes: (1) Combustion Process I, (2) Combustion Process II and (3) Thermodynamic Functions. Input and output data are on cards. However, the final solution to a problem will be typed out on the 1620 console typewriter.

THERMODYNAMIC FUNCTIONS

PROGRAM DESCRIPTION

The program calculates thermodynamic data at any temperature T (ranging from 300°-3500° K) for use in the Combustion Process I Program.

Thermodynamic data obtained from the program will be the following:

(1) C_p^o - specific heat at constant pressure and standard conditions. cal./(mole, °K)

(2) H_T^o - sum of sensible enthalpy and chemical energy at temperature T and standard conditions. (Kcal/mole)

(3) $\frac{\Delta H}{RT}$ - enthalpy change divided by gas constants times temperature multiplied by -1.

(4) Log K - logarithm of equilibrium constant.

(5) S_T^o * - molar entropy at standard conditions. cal./(mole, °K)

* S_T^o is included in the output but is not used in the Combustion Program.

Input data to the program are the Coefficients of Thermodynamic Tables II, III, and IV. Further discussion of the tables will be given under the sections entitled "Mathematics" and "Restrictions".

All input and output data in the program will be on cards.

COMBUSTION PROCESS I

PROGRAM DESCRIPTION

Combustion Process I sets up an X-matrix and Y-matrix which are used in Combustion Process II to solve for new estimates of "P_i". The program also sets up an error parameter, "e", and tests to see whether or not "e" is less than or equal to .0015. Whenever the value of "e" is greater than .0015, it is concluded that the desired values of the partial pressure, temperature and the formula weight of the reactants have not been reached. Therefore, the program will type out a message to load Combustion Process II. If the value of "e" is less than or equal to .0015, the desired values have been reached, and the program will type out the partial pressures, "P_i", the equilibrium temperature, T, and the number of formula weights of the reactants in an E 14.8 format.

The maximum numbers of compounds and elements that may be processed through the program are thirteen (13) and seven (7), respectively. A control card which tells the processor the number of compounds and the number of elements involved in a problem will enable the program to process any number of compounds less than or equal to thirteen and any number of elements less than or equal to seven.

COMBUSTION PROCESS II

PROGRAM DESCRIPTION

Combustion Process II calculates new estimates for input into Combustion Process I and a new temperature for input into the Thermodynamic Functions Program.

Input data for the program are: (1) one control card, and (2) the X-matrix and Y-matrix left in the machine from Combustion Process I.

Output data will be on cards and will be in the following order:

Temperature Card

Control Data Card

A, P, T Card

Log P(i) Data Cards

MATHEMATICS AND/OR TECHNIQUES

The method used in the program for the computation of equilibrium temperatures and compositions of adiabatic combustion reactions was devised by Huff, Gordon and Morrell.(1) A set of equations, representing dissociative equilibria, pressure balance, mass balance and energy balance is solved simultaneously by successive iterations of a series of correction equation. Each of these correction equations contains a correction variable which takes the form:

$$\delta x = \Delta x \log \frac{X_o}{X} \quad (1)$$

Due to the limited storage capacity of the 1620 computer and the necessity to calculate thermodynamic data for each iteration, the program is written in three parts. The function of each part is as follows:

(1) Using the estimates of the partial pressures of the reactants involved in the combustion process, thermodynamic properties determined by the Thermodynamic Functions Program, an estimated temperature, the general formula and total enthalpy as basic data, Combustion Process I (Deck 1) constructs two matrices in the manner described by Huff, Gordon and Morrell,(1) and tests for convergence using .0015 as the tolerance level.

(2) Combustion Process II (Deck 2) multiplies the two matrices that were constructed in Combustion Process I and computes new estimates from the matrix obtained as a result of the matrix multiplication by using the Crout(2) method for solving a matrix, as suggested by Huff, Gordon and Morrell.(1)

(3) The Thermodynamic Functions Program (Deck 3) computes the thermodynamic properties given in equations (2) - (6) for use in the Combustion Process I Program (Deck 1). The coefficients and constants in Tables II, III and IV used in computing the thermodynamic properties necessary for Combustion Process I were computed specifically for the purpose of being used with the Thermodynamic Functions Program. The following equations representing the molar specific heat, the molar enthalpies, the molar entropies, the enthalpy change and the equilibrium constant are used in the program:

$$C_p^o = \alpha + \beta T + \gamma T^2 + \delta T^3 \quad (2)$$

$$H_T^o = (\alpha T + 1/2\beta T^2 + 1/3\gamma T^3 + 1/4\delta T^4)\, 10^{-3} + C \quad (3)$$

$$S_T^o = \alpha \ln T + \beta T + 1/2\gamma T^2 + 1/3\delta T^3 + K \quad (4)$$

$$\frac{\Delta H}{RT} = a + bT + cT^2 + dT^3 + \frac{m}{T \times 10^{-3}} \quad (5)$$

$$\text{Log } K = A \log T + BT + \Gamma T^2 + \Delta T^3 + L + \frac{M}{T \times 10^{-3}} \quad (6)$$

Data contained in the National Aeronautics and Space Administration Report (3) were used to determine the coefficients in equations (2) - (6). However, applying equation (1) to the conservation of energy:

$$S_h = Ah \log \frac{h_o}{h} \quad (7)$$

where "h_o" is the enthalpy of the reactants and "h" is the sum of the enthalpies of the product weighted by their respective mole fraction of the combustion products. If for any reason, the values of "h_o" and "h" would be opposite in sign, the expression containing the log (h_o/h) would create an error response in the computer. Therefore, to evaluate "C" of equation (3), assigned enthalpies, as shown in Table I, were used.

TABLE I

ENTHALPY ASSIGNED TO SEVERAL SUBSTANCES

Element	Phase	H_{298}
Ar	Gas	1.4812
Br_2	Liquid	2.6600
C	Graphite	92.1790
H_2	Gas	69.4407
N_2	Gas	3.7715
O_2	Gas	4.1109
S	Rhombic	100.0000

REFERENCES

(1) Huff, Y. N., Gordon, S., Morrell, V. E., - "General Method and Thermodynamic Tables for Computation of Equilibrium Composition and Temperature of Chemical Reactions", NACA, Report 1037 (1951).

(2) Crout, P.D., - "A Short Method for Evaluating Determinants and Solving Systems of Linear Equations with Real or Complex Coefficients", Trans. Amer. Inst. Elec. Engs., 60 (1941).

(3) McBride, B. J., Heimel, S., Ehlers, J. G., Gordon, S., - "Thermodynamic Properties to 6000° K for 210 Substance Involving the First 18 Elements", NASA, Sp-3001, (1963).

INPUT AND OUTPUT FORMATS

INPUT/OUTPUT FORMAT
THERMODYNAMIC FUNCTIONS

INPUT/OUTPUT FORMATS

THERMODYNAMIC FUNCTIONS

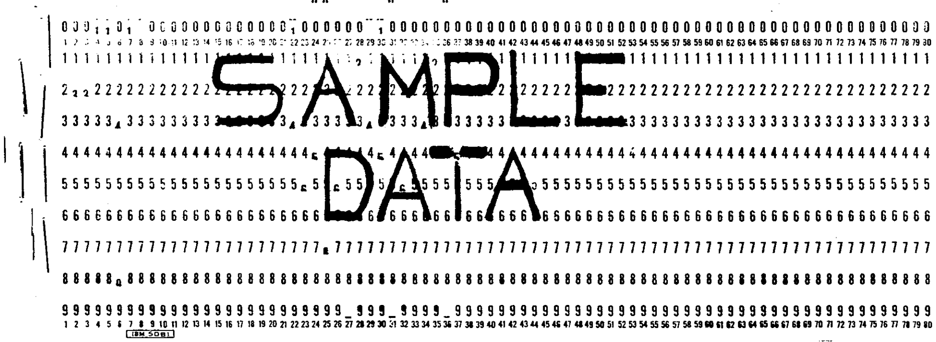
Input

A set of input data for a compound or element being processed through the Thermodynamic Functions Program consists of three cards (one from each of the Coefficients of Thermodynamic Functions Tables). A 2, 3 or 4 will be punched in Column 80 for Tables II, III or IV, respectively. A set of data being processed **must** be in numeric order by table code.

All data being processed are preceded by a temperature card. The temperature card will be the first card read into the program and will have the following format:

Description	Columns	FORTRAN Symbol	Format
T (°K)	1-8	T	F8.2

```
-503059  069916 -006240  000319   385222 4775775          H20     4
 503059 -160988  028738 -002206 10996629                  H20     3
 495233  638682 -172814  018124  1230309 1580923          H20     2
  -207869  016067 -000377 -000032   090789 2246215          H2      4
   207869 -036996  001736  000218  5172101                  H2      3
   580531  147043 -010349 -001733  6768494 -180405          H2      2
  2200.00            TEMPERATURE CARD
```



Input data from all three tables are on cards and will be in the following formats:

Table II

Description	Columns	FORTRAN Symbol	Format
α	1-8	A	F8.5
$\beta \times 10^3$	9-16	B	F8.5
$\gamma \times 10^6$	17-24	CC	F8.5
$\delta \times 10^9$	25-32	D	F8.5
C	33-41	E	F9.5
K	42-49	F	F8.5
Identification	55-57	ID	I2
Table Code	80		

Table III

Description	Columns	FORTRAN Symbol	Format
a	1-8	AA	F8.5
$b \times 10^3$	9-16	BB	F8.5
$c \times 10^6$	17-24	CCC	F8.5
$d \times 10^9$	25-32	DD	F8.5
m	33-41	EE	F9.5
Table Code	80		

Table IV

Description	Columns	FORTRAN Symbol	Format
A	1-8	AAA	F8.5
$B \times 10^3$	9-16	BBB	F8.5
$C \times 10^6$	17-24	CK	F8.5
$\Delta \times 10^9$	25-32	DDD	F8.5
L	33-41	EEE	F9.5
M	42-49	F	F8.5
Table Code	80		

Output

All output data are on cards. There will be one card punched for each set of data read. The order of the elements and compounds in the output is the same as their original order in the input.

The output format will be as follows:

Description	Columns	FORTRAN Symbol	Format
C_p^o cal./(mole, °K)	1-9	C	F9.4
H_T^o (Kcal/mole)	10-18	H	F9.4
$\frac{\Delta H}{RT}$	19-27	HH	F9.4
log K	28-36	CECF	F9.4
S_T^o cal./(mole, °K)	37-45	S	F9.4
Identification	76-80	ID	I5

SAMPLE INPUT DATA

FOR

THERMODYNAMIC FUNCTIONS PROGRAM

2200.00 TEMP. = 2200 K

580531	147043	-010349	-001733	6768494	-180405	H2	2
207869	-036996	001736	000218	5172101		H2	3
-207869	016067	-000377	-000032	090789	2246215	H2	4
495233	638682	-172814	018124	1230309	1580923	H2O	2
503059	-160988	028738	002206	10996629		H2O	3
-503059	069916	-006240	000319	385222	4775775	H2O	4
538982	243528	-061041	005829	4467687	1312034	OH	2
231047	-061566	009990	-000659	5073363		OH	3
-231047	026738	-002169	000095	188357	2203334	OH	4
963218	502247	-176740	022673	141059	-643266	CO2	2
279290	-134150	031209	-002810	19305350		CO2	3
-279290	058261	-006777	000407	-639973	8384207	CO2	4
620126	255577	-088801	011249	6578319	1103990	CO	2
199668	-071794	016708	-001447	12896790		CO	3
-199668	031180	-003628	000210	-074022	5601005	CO	4
595705	271090	-092791	011599	186228	1106826	N2	2
192766	-061552	012924	-001065	11325067		N2	3
-192766	026732	-002806	000154	-055680	4918414	N2	4
664779	221014	-077591	009955	2332637	1159108	NO	2
164012	-052574	011446	-000981	7562922		NO	3
-164012	022832	-002485	000142	-084787	3284535	NO	4
761206	094407	-016012	002108	148991	472934	O2	2
121493	-024340	002188	-000117	5979684		O2	3
-121493	010571	-000475	000017	-281254	2596944	O2	4
606270	702346	-230861	028578	16243440	1252268	H2S	2
482659	-200597	045752	-004241	8708322		H2S	3
-482659	087118	-009935	000614	351185	3781976	H2S	4
848089	053176	-017635	002345	22811776	564902	S2	2
148721	-061149	017015	-001596	5108413		S2	3
-148721	026557	-003695	000230	-156036	2218556	S2	4
1110546	292319	-103367	013607	2911630	-613302	SO2	2
33444	-098020	023869	-002209	12883220		SO2	3
-233444	042570	-005183	000320	-642058	5595112	SO2	4
1523516	460266	-171284	022566	589454	-2908528	SO3	2
277904	-140570	035012	-003261	17079080		SO3	3
-277904	061049	-007603	000472	-1343033	7417350	SO3	4
496810	000000	000000	000000	8533690	-091377	H	2
						H	3
						H	4
515597	-028602	012290	-000845	26191504	838824	C	2
						C	3
						C	4
489391	013226	-007869	001568	11346040	872343	N	2
						N	3
						N	4
496810	000000	000000	000000	000000	867698	AR	2
						AR	3
						AR	4
501322	-001167	-001484	000591	6016089	1000671	O	2
						O	3
						O	4
571818	-094930	041903	-005130	16481760	787223	S	2
						S	3
						S	4

INPUT/OUTPUT FORMAT
COMBUSTION PROCESS I

INPUT/OUTPUT FORMATS

COMBUSTION PROCESS I

Input

A set of input data into Combustion Process I will be in the following format and order:

1. Control Data Card (One Card)

Card Column		Format	FORTRAN Symbol
1-3	Number of Compounds	I3	N
4-5	Number of Elements	I2	M
78-80	101 (Identification No.)		

2. A, P, T Data Card (One Card)

Card Column		Format	FORTRAN Symbol
1-14	Number of Formula Weights of Reactants	E14.7	B(1)
15-28	Initial Estimate of Total Pressure	E14.7	P(1)
29-42	Temperature	E14.7	T(1)
78-80	201 (Identification No.)		

3. Log P(i) Data Cards (No. of Cards Determined by No. of Reactants)

Card Column		Format	FORTRAN Symbol
1-14	Log P(i)	E14.6	X(8,i)
78-80	301, 302, Etc. (Identification No.)		

4. Thermodynamic Data Cards (No. of Cards Determined by No. of Reactants)

Card Column		Format	FORTRAN Symbol
1-9	C^o_p	F9.4	X(1,I)
10-18	H^o_T	F9.4	X(9,I)
19-27	$\Delta H/RT$	F9.4	Y(9,I)
28-36	Log K_i	F9.4	Y(10,I)
37-45	S^o_T	F9.4	
78-80	401, 402, Etc.		

5. a_o, b_o, ..., h_o Data Card (One Card)

Card Column		Format	FORTRAN Symbol
1-9	a_o - No. of Atoms of Respective Element in Formula	F9.4	O(1)
10-18	b_o - No. of Atoms of Respective Element in Formula	F9.4	O(2)
19-27	c_o - No. of Atoms of Respective Element in Formula	F9.4	O(3)
28-36	d_o - No. of Atoms of Respective Element in Formula	F9.4	O(4)
37-45	e_o - No. of Atoms of Respective Element in Formula	F9.4	O(5)
46-54	f_o - No. of Atoms of Respective Element in Formula	F9.4	O(6)
55-63	g_o - No. of Atoms of Respective Element in Formula	F9.4	O(7)
64-72	h_o - Initial Enthalpy per Mole of Reactants	F9.4	O(8)
78-80	501 (Identification No.)		

6. a_i, b_i, . . ., g_i Data Card (No. of Cards Determined by No. of Reactants)

1-9	a_i - No. of Atoms per Element in Reactant Product	F9.4	Y(1,i)
10-18	b_i - No. of Atoms per Element in Reactant Product	F9.4	Y(2,i)

6. a_i, b_i, . . ., g_i Data Card (No. of Cards Determined by No. of Reactants) (Cont.)

Card Column		Format	FORTRAN Symbol
19-27	c_i - No. of Atoms per Element in Reactant Product	F9.4	Y(3,i)
28-36	d_i - No. of Atoms per Element in Reactant Product	F9.4	Y(4,i)
37-45	e_i - No. of Atoms per Element in Reactant Product	F9.4	Y(5,i)
46-54	f_i - No. of Atoms per Element in Reactant Product	F9.4	Y(6,i)
55-63	g_i - No. of Atoms per Element in Reactant Product	F9.4	Y(7,i)
78-80	601, 602, Etc. (Identification No.)		Q(i)

Output

Output data for Combustion Process I will be from the typewriter if the error parameter "E" is less than or equal to .0015. If E is greater than .0015, the data in core store are left in the machine and are used as data for Combustion Process II. The typewriter will type out the following message:

"Push reset, Load Combust. Prog. 2."

A sample output listing of Combustion Process I is shown on the next page.

SAMPLE OUTPUT

COMBUSTION PROCESS I

H2	.11437648E-Ø2
H2O	.73Ø96864E-Ø1
OH	.23769886E-Ø2
CO2	.1516684ØE ØØ
CO	.1278Ø94E-Ø1
N2	.735629Ø2E ØØ
NO	.29623556E-Ø2
O2	.92114445E-Ø2
H2S	.176413Ø3E-Ø8
S2	.2Ø187753E-1Ø
SO2	.17414738E-Ø2
SO3	.5Ø23117ØE-Ø6
H	.2433694ØE-Ø3
C	.32717617E-16
N	.17737Ø53E-Ø7
AR	.88Ø19261E-Ø2
O	.34Ø69531E-Ø3
S	.5825Ø858E-Ø7

A= .3Ø5619ØØE ØØ

T= .224487ØØE Ø4

STOP ØØØØ

INPUT/OUTPUT FORMAT
COMBUSTION PROCESS II

INPUT/OUTPUT FORMAT

COMBUSTION PROCESS II

Input

Combustion Process II requires only one data card. The data card is a control card and has the following format:

Card Column		Format
1-3	No. of Compounds	I3
4-5	No. of Elements	I2

Output

Output data will be on cards and will have the following format:

Card Column		Format	FORTRAN Symbol
1. Temperature Card			
1-8		F8.2	T(1)
2. Control Data Card			
1-3	No. of Compounds	I3	N
4-5	No. of Elements	I2	M
78-80	101 (Identification No.)		
3. A, P, T Data Card (One Card)			
1-14	No. of Formula Weights of Reactants	E14.7	B(1)
15-28	Initial Estimate of Total Pressure	E14.7	P(1)
29-42	Temperature	E14.7	T(1)
78-80	201 (Identification No.)		
4. Log P(i) Data Cards (No. of Cards Determined by No. of Reactants)			
1-14	Log P(i)	E14.6	X(8,i)
78-80	301, 302, Etc. (Identification No.)		

RESTRICTIONS

RESTRICTIONS

The program is restricted to computation for adiabatic chemical reactions in which the total number of compounds and elements does not exceed 13 and 7, respectively. A code card will allow any variable number of compounds and elements to be processed. (For example, 5 compounds and 2 elements, 11 compounds and 5 elements, 12 compounds and 7 elements, etc.) The code card is also used to avoid division by zero and to avoid the possibility of taking the log of a zero quantity.

In the test for convergence, the program requires that ϵ * $\leq$ .0015. However, the smaller the value of ϵ, the more accurate the final results will be. Thus, for a greater degree of accuracy the user of the program may want to require ϵ to be smaller than .0015.

The coefficients and constants in Tables II, III and IV used to determine thermodynamic properties are limited to a total number of seven elements and seventeen molecular or radical species. If thermodynamic data for other species are required, the coefficients and constants in equations (1) - (5) may be determined by referring to reference (3). However, to determine "C" in equation (2), reference should always be made to the assigned enthalpies in Table I. If an element not listed in Table I should be involved, a value may be assigned to represent its molar enthalpy in its standard state. The assigned value should be selected so as to result only in positive values of enthalpy for all other species containing this particular element.

The constants and coefficients in Tables II, III and IV are for use only with the Thermodynamic Functions Program submitted with this writeup. The thermodynamic values obtained from the program by the use of these equations are not internally consistent with values obtained from other sources.

If the original estimates are too unreasonable, the results obtained in any given iteration may exceed, in temperature, the thermodynamic equations furnished with this program. In such cases, it is suggested the program be reconsidered with more reasonable estimates.

* - The FORTRAN symbol for ϵ is E.

OPERATING INSTRUCTIONS

OPERATING INSTRUCTIONS

THERMODYNAMIC FUNCTIONS

Sorting Input

Input data are in the order as indicated in the Input/Output Formats for Thermodynamic Functions Program. No further sorting is required.

Clearing Core

The Object Deck, which was compiled by PDQ FORTRAN, automatically clears core when it is loaded in the machine.

Switch Settings

All program switches are set to "off".

Loading Object Deck and Data

Place Object Deck in 1622 read hopper, followed by temperature card and data punched from Thermodynamics Coefficients Table.* Push "load" button.

Program Stops

There are no "halts" in the program.

Output Data

All output data are on cards and require no sorting. After all input data have been processed, the machine's "reader no feed" light will be on. Retain output data for input into Combustion Process I Program.

*Note: The set of data used depends on the temperature. Each time a new temperature is used, the program must be reloaded, followed by the temperature card and data from the tables for that particular temperature range.

OPERATING INSTRUCTIONS

COMBUSTION PROCESS I

Sorting Input

Input data are in the order as indicated in the Input/Output Formats for Combustion Process Program I. No further sorting is required.

Clearing Core

The Object Deck, which was compiled by PDQ FORTRAN, automatically clears core when it is loaded in the machine.

Switch Settings

All program switches are set to "off".

Operation (1st Iteration)

1. All data for the first run should be carefully edited.

2. Load Object Deck.

3. Load data.

4. If the following message is typed out on the typewriter:

   "Push reset, Load Combust. Prog. 2."

   Do not clear the machine. Push reset and load Combustion Process II. If the desired answers to the problem have been obtained, the final answers will be typed out on the typewriter in the format indicated in the writeup under Input/Output Formats for Combustion Process I. Processing will then be complete.

Operation (2nd Iteration)

1. Remove first four sets of original input data.

2. Replace original data with new data obtained from Combustion Process II, followed by new data obtained from Thermodynamic Functions Program.

3. Repeat Steps 2 - 4 of first iteration.

Operation (3rd, 4th, 5th, Etc. Iterations)

1. "Same as second iteration".

Program Stops

The program will come to a halt only when processing is complete.

OPERATING INSTRUCTIONS

COMBUSTION PROCESS II

Input Data

Input data are left in machine from Combustion Process I. One data card (control data card) is also read in as input to the program.

"Do not clear machine before loading Program".

Loading Program

When message is typed out from Combustion Process I, the program will come to a halt. Push reset and load program with data control input card on back.

Output

All output data are on cards. Retain temperature card (1st output data card) for processing through Thermodynamic Functions Program. The remaining data will be processed through Combustion Process I.

Program Stops

The program comes to a halt only when processing is complete.

SUPPORTING DOCUMENTATION AND MATERIALS

SAMPLE PROBLEMS

SAMPLE PROBLEM NO. 1

INPUT DATA

```
 8 5
0.0000001E+07 0.0000001E+07 0.0002200E+07
-3.000000E+00                                                    H2
-2.732828E+00                                                    H2O
-2.698970E+00                                                    OH
-2.031517E+00                                                    CO2
-2.698970E+00                                                    CO
-2.148742E+00                                                    N2
-3.000000E+00                                                    NO
-3.000000E+00                                                    O2
-4.000000E+00                                                    H
-15.000000E+00                                                   C
-6.000000E+00                                                    N
-2.096910E+00                                                    AR
-4.000000E+00                                                    O
  8.3548  83.5462 -24.8815   4.5019  45.7977
 12.5689  33.5819 -53.0993  10.0160  64.4355
  8.4137  60.6026 -24.4301   4.6695  58.6888
 14.5416  29.8104 -88.8044  23.3723  75.2756
  8.7237  83.1178 -59.6935  18.5778  62.6390
  8.6650  18.9139 -52.5632  15.8252  61.0450
  8.8147  41.1290 -35.3099   8.9970  66.0917
  9.1384  20.0762 -27.9532   5.1423  65.0775
  4.9681  96.2667   -.0000    .0000  37.3217
  5.0315 272.9527   -.0000    .0000  47.7078
  4.9709 124.3596   -.0000    .0000  46.5441
  4.9681  10.9298   -.0000    .0000  46.9124
  4.9786  71.1436   -.0000    .0000  48.5488
```

4.0000	1.0029	14.9098	0.0890	4.0057	249.6473	
2.0000						H2
2.0000				1.0000		H2O
1.0000				1.0000		OH
	1.0000			2.0000		CO2
	1.0000			1.0000		CO
		2.0000				N2
		1.0000		1.0000		NO
				2.0000		O2
1.0000						H
	1.0000					C
		1.0000				N
			1.0000			AR
				1.0000		O

SAMPLE PROBLEM NO. 1

ANSWERS

H2	.33758818E-Ø2
H2O	.18343331E ØØ
OH	.26925Ø9ØE-Ø2
CO2	.86Ø85267E-Ø1
CO	.83511769E-Ø2
N2	.7Ø1Ø6510E ØØ
NO	.18175524E-Ø2
O2	.42697982E-Ø2
H	.342Ø2367E-Ø3
C	.15Ø1ØØ15E-16
N	.11329261E-Ø7
AR	.838Ø65ØØE-Ø2
O	.1851Ø828E-Ø3

A= .94163ØØØE-Ø1

T= .22Ø85ØØØE Ø4

STOP ØØØØ

SAMPLE PROBLEM NO. 2

INPUT DATA

12 6

.0000031E+05 0.0000001E+07 0.0002200E+07

-2.52288E+00

-1.22185E+00

-2.69897E+00

-0.82391E+00

-1.69897E+00

-0.15490E+00

-2.69897E+00

-2.30103E+00

-6.00000E+00

-6.00000E+00

-2.69897E+00

-6.00000E+00

-3.39794E+00

-17.0000E+00

-5.30103E+00

-2.05061E+00

-3.69897E+00

-8.00000E+00

8.3548	83.5462	-24.8815	4.5019	45.7977
12.5689	33.5819	-53.0993	10.0160	64.4355
8.4137	60.6026	-24.4301	4.6695	58.6888
14.5416	29.8104	-88.8044	23.3723	75.2756
8.7237	83.1178	-59.6935	18.5778	62.6390
8.6650	18.9139	-52.5632	15.8252	61.0450
8.8147	41.1290	-35.3099	8.9970	66.0917

9.1384	20.0762	-27.9532	5.1423	65.0775			
13.3836	186.2487	-41.7595	6.0712	70.0615			
9.0469	247.5739	-24.0155	3.9830	71.7460			
13.9823	57.7504	-59.6581	11.9288	83.7493			
19.4736	45.7924	-78.6660	12.0215	94.9493			
4.9681	96.2667	-.0000	.0000	37.3217			
5.0315	272.9527	-.0000	.0000	47.7078			
4.9709	124.3596	-.0000	.0000	46.5441			
4.9681	10.9298	-.0000	.0000	46.9124			
4.9786	71.1436	-.0000	.0000	48.5488			
5.1115	176.2871	-.0000	.0000	50.6240			
0.4944	0.5381	4.8237	0.0288	1.3638	0.0057	75.8600	
2.0000							H2
2.0000				1.0000			H2O
1.0000				1.0000			OH
	1.0000			2.0000			CO2
	1.0000			1.0000			CO
		2.0000					N2
		1.0000		1.0000			NO
				2.0000			O2
2.0000					1.0000		H2S
					2.0000		S2
				2.0000	1.0000		SO2
				3.0000	1.0000		SO3
1.0000							H
	1.0000						C
		1.0000					N
			1.0000				AR
				1.0000			O
					1.0000		S

SAMPLE PROBLEM NO. 2

ANSWERS

```
H2     .11437648E-Ø2
H2O    .73Ø96864E-Ø1
OH     .23769886E-Ø2
CO2    .1516684ØE ØØ
CO     .127860934E-Ø1
N2     .735629Ø2E ØØ
NO     .29623556E-Ø2
O2     .92114445E-Ø2
H2S    .176413Ø3E-Ø8
S2     .2Ø187753E-1Ø
SO2    .17414738E-Ø2
SO3    .5Ø23117ØE-Ø6
H      .2433694ØE-Ø3
C      .32717617E-16
N      .17737Ø53E-Ø7
AR     .88Ø19261E-Ø2
O      .34Ø69531E-Ø3
S      .5825Ø858E-Ø7

A= .3Ø5619ØØE ØØ
T= .224487ØØE Ø4
STOP ØØØØ
```


SOURCE PROGRAM LISTINGS

PROGRAM LISTING

THERMODYNAMIC FUNCTIONS

```
26ØØØØ8ØØØØ9RS
PDQ FORTRAN C2
START

-66ØØ        READ 3Ø, T
-6624      5 READ 1Ø, A,B,CC,D,E,F,ID
-672Ø        B=B/1Ø.**3.
-6768        CC=CC/1Ø.**6.
-6816        D=D/1Ø.**9.
-6864        X=Ø.434294*LOG(T)
-69ØØ        C=A+B*T+CC*T**2.+D*T**3.
-7Ø68        H=((A*T+.5*B*T**2.+CC*T**3./3.+.25*D*T**4.)/1Ø.**3.)+E
-7428        S=2.3Ø2585*A*X+B*T+.5*CC*T**2.+D*T**3./3.+F
-77Ø4        READ 1Ø, AA,BB,CCC,DD,EE
-7776        BB=BB/1Ø.**3.
-7824        CCC=CCC/1Ø.**6.
-7872        DD=DD/1Ø.**9.
-792Ø        HH=AA+BB*T+CCC*T**2.+DD*T**3.+(EE/(T*1Ø.**-3.))
-816Ø        HH=(-1.)*HH
-82Ø8        READ 1Ø, AAA,BBB,CK,DDD,EEE,FF
-8292        BBB=BBB/1Ø.**3.
-834Ø        CK=CK/1Ø.**6.
-8388        DDD=DDD/1Ø.**9.
-8436        CECF=AAA*X+BBB*T+CK*T**2.+DDD*T**3.+EEE+(FF/(T*1Ø.**-3.))
-8724        ID=ID+4ØØ
-876Ø        PUNCH 2Ø, C,H,HH,CECF,S,ID
-8844        GO TO 5
-8852     1Ø FORMAT (4F8.5,F9.5,F8.5,5X,I2)
```



```
-8912     2Ø FORMAT (5F9.4,3ØX,I5)
-8966     3Ø FORMAT (F8.2)
-8988        END
T9999 SIN
T9989 SINF
T9979 COS
T9969 COSF
T9959 EXP
T9949 EXPF
T9939 LOG
T9929 LOGF
T9919 SQRT
T99Ø9 SQRTF
T9899 ABS
T9889 ABSF
T9879 DRH
T9869 DRHF
T9859 ATAN
T9849 ATANF
T9839 ØØ3Ø
T9829 T
T9819 ØØØ5
T98Ø9 ØØ1Ø
T9799 A
T9789 B
T9779 CC
T9769 D
T9759 E
T9749 F
T9739 ID
T9729 521ØØØØØØØ
T9719 513ØØØØØØØ
T97Ø9 ØØØ
```

```
T9699 516ØØØØØØØ
T9689 519ØØØØØØØ
T9679 X
T9669 5Ø434294ØØ
T9659 C
T9649 512ØØØØØØØ
T9639 ØØ1
T9629 ØØ2
T9619 H
T96Ø9 5Ø5ØØØØØØØ
T9599 ØØ3
T9589 ØØ4
T9579 ØØ5
T9569 5Ø25ØØØØØØ
T9559 ØØ6
T9549 514ØØØØØØØ
T9539 ØØ7
T9529 ØØ8
T9519 S
T95Ø9 5123Ø2585Ø
T9499 AA
T9489 BB
T9479 CCC
T9469 DD
T9459 EE
T9449 HH
T9439 511ØØØØØØØ
T9429 AAA
T9419 BBB
T94Ø9 CK
T9399 DDD
T9389 EEE
T9379 FF
```



```
T9369 CLCF
T9359 Ø4ØØ
T9349 ØØ2Ø
```

LOAD SUBROUTINES

```
26ØØØØ8ØØØØ9RS
```

PROGRAM LISTING

COMBUSTION PROCESS I

```
PDQ FORTRAN C2
START
-66ØØ  C     COMBUSTION PROCESS
-66ØØ  C     PROGRAMMED FOR RESEARCH DEPARTMENT
-66ØØ  C     OCTOBER, 1964
-66ØØ        DIMENSION X(9,23),Y(1Ø,23),B(1),P(1),T(1),O(8),Z(9),Q(2Ø)
-66ØØ        READ 6Ø,N,M
-6636        M=M+13
-6672        DO 99 I=1,9
-6684        Z(I)=Ø.
-672Ø        DO 99 J=1,23
-6732     99 X(I,J)=Ø.
-6876        DO 3Ø I=1,1Ø
-6888        DO 3Ø J=1,23
-69ØØ     3Ø Y(I,J)=Ø.
-7Ø44        READ 4Ø2,B(1),P(1),T(1)
-7Ø92        DO 4ØØ I=1,N
-71Ø4    4ØØ READ 4Ø2,X(8,I)
-7212        DO 4Ø3 I=14,M
-7224    4Ø3 READ 4Ø2,X(8,I)
-7332        K=1
-7344        L=N
-7356      8 DO 9 I=K,L
-7368      9 READ 1ØØ,X(1,I),X(9,I),Y(9,I),Y(1Ø,I)
-7656        IF (L-N) 1Ø,11,1Ø
-7724     11 K=14
-7736        L=M
-7748        GO TO 8
-7756     1Ø READ 1ØØ,O(1),O(2),O(3),O(4),O(5),O(6),O(7),O(8)
-7864        DO 4Ø4 I=1,N
-7876    4Ø4 X(8,I)=EXP((X(8,I)/.434294))
-8Ø56        DO 4Ø5 I=14,M
-8Ø68    4Ø5 X(8,I)=EXP((X(8,I)/.434294))
-8248        DO 13 I=1,2Ø
-826Ø        X(9,22)=X(9,22)+X(8,I)*X(1,I)
-84Ø4        X(9,I)=X(8,I)*X(9,I)
-8584        X(9,21)=X(9,21)+X(9,I)
-8668     13 CONTINUE
-87Ø4        X(9,22)=T(1)*X(9,22)/1ØØØ.
-8752        X(9,21)=(-1.)*X(9,21)
-88ØØ        K=1
-8812        L=N
-8824     2Ø DO 14 I=K,L
-8836     14 READ 6ØØ,Y(1,I),Y(2,I),Y(3,I),Y(4,I),Y(5,I),Y(6,I),Y(7,I),Q(I)
-934Ø        IF (L-N) 15,17,15
-94Ø8     17 K=14
-942Ø        L=M
-9432        GO TO 2Ø
-944Ø     15 DO 16 I=1,7
-9452        DO 16 J=1,2Ø
-9464        X(I,J)=X(8,J)*Y(I,J)
-9668     16 X(I,21)=X(I,21)+X(I,J)
-9884        DO 18 I=1,7
-9896     18 X(I,21)=X(I,21)*(-1.)
JØØ28        DO 19 I=1,1Ø
JØØ4Ø     19 Y(I,I+13)=1.
JØ148        M=M-13
JØ184        DO 41 J=1,N
JØ196        Y(1Ø,J)=-Y(1Ø,J)+(LOG(X(8,J))*.434294)
JØ388        DO 41 I=1,M
JØ4ØØ     41 Y(1Ø,J)=Y(1Ø,J)-Y(I,J)*(LOG(X(8,I+13))*.434294)
JØ748  C     SUM P(I)
```

```
J0748        SUMP=0.
J0760        V=0.
J0772        DO 51 I=1,20
J0784        V=V+ABS(Y(10,I))
J0868     51 SUMP=SUMP+X(8,I)
J0988        DO 74 I=1,M
J1000     74 Z(I)=LOG(B(I)*O(I)/((-1.)*X(I,21)))*.434294
J1228        Z(8)=LOG(B(1)*O(8)/((-1.)*X(9,21)))*.434294
J1348        Z(9)=LOG(P(1)/SUMP)*.434294
J1408        DO 50 I=1,M
J1420     50 X(I,23)=(-1.)*X(I,21)*Z(I)
J1588        X(8,23)=SUMP*Z(9)
J1624        X(9,23)=(-1.)*X(9,21)*Z(8)
J1684        L=M
J1696        M=M+13
J1732        E=V
J1744        DO 83 I=1,9
J1756     83 E=E+ABS(Z(I))
J1852        IF (E-.0015) 200,200,201
J1920    200 DO 210 I=1,N
J1932    210 TYPE 202,Q(I),X(8,I)
J2076        DO 310 I=14,M
J2088    310 TYPE 202, Q(I),X(8,I)
J2232        TYPE 205,B(1),T(1)
J2268        STOP
J2280    201 TYPE 212
J2292    212 FORMAT(/34HPUSH RESET. LOAD COMBUST. PROG. 2.)
J2390        STOP
J2402     60 FORMAT (I3,I2)
J2430    402 FORMAT (3E14.0)
J2462    600 FORMAT (7F9.4,9X,A4)
J2526    100 FORMAT (8F9.4)
J2584    202 FORMAT (/A4,3H    ,E14.8)
```



```
J2630    205 FORMAT (//2HA=,E14.8/,2HT=,E14.8)
J2694        END
T9999 SIN
T9989 SINF
T9979 COS
T9969 COSF
T9959 EXP
T9949 EXPF
T9939 LOG
T9929 LOGF
T9919 SQRT
T9909 SQRTF
T9899 ABS
T9889 ABSF
T9879 DRH
T9869 DRHF
T9859 ATAN
T9849 ATANF
T9839 X      T7779
T7769 Y      T5479
T5469 B      T5469
T5459 P      T5459
T5449 T      T5449
T5439 O      T5369
T5359 Z      T5279
T5269 Q      T5079
T5069 0060
T5059 N
T5049 M
T5039 0013
T5029 000
T5019 0099
T5009 I
```

```
T4999 ØØØØØØØØØØ
T4989 J
T4979 ØØ3Ø
T4969 Ø4Ø2
T4959 Ø4ØØ
T4949 Ø4Ø3
T4939 K
T4929 ØØØ1
T4919 L
T4909 ØØØ8
T4899 ØØØ9
T4889 Ø1ØØ
T4879 ØØ1Ø
T4869 ØØ11
T4859 ØØ14
T4849 Ø4Ø4
T48 9 5Ø43429400
T4829 ØØ1
T4819 Ø4Ø5
T4809 ØØ13
T4799 541ØØØØØØØ
T4789 511ØØØØØØØ
T4779 ØØ2Ø
T4769 ØØ14
T4759 Ø6ØØ
T4749 ØØ15
T4739 ØØ17
T4729 ØØ16
T4719 ØØ18
T4709 ØØ19
T4699 ØØ41
T4689 SUMP
T4679 V
```



```
T4669 ØØ51
T4659 ØØ74
T4649 ØØ3
T4639 ØØ5Ø
T4629 E
T4619 ØØ83
T4609 4815ØØØØØØ
T4599 Ø2ØØ
T4589 Ø2Ø1
T4579 Ø21Ø
T4569 Ø2Ø2
T4559 Ø31Ø
T4549 Ø2Ø5
T4539 Ø212

LOAD SUBROUTINES
PDQ FIXED FMT SUBROUTNS 11/63
PROCESSING COMPLETE
```

PROGRAM LISTING

COMBUSTION PROCESS II

```
26ØØØØ8ØØØØ9RS
PDQ FORTRAN C2
START
-66ØØ  C    SECOND PART OF COMBUSTION PROGRAM
-66ØØ  C    NOVEMBER 6, 1964
-66ØØ       DIMENSION X(9,23),Y(1Ø,23),A(1),C(1),T(1),R(9,1Ø),P(2Ø),V(9)
-66ØØ       READ 2ØØ,N,M
-6636  C    MULTIPLY X MATRIX BY Y MATRIX
-6636       DO 22 I=1,9
-6648       DO 22 K=1,1Ø
-666Ø       R(I,K)=Ø.
-6732       DO 22 J=1,23
-6744    22 R(I,K)=R(I,K)+X(I,J)*Y(K,J)
-714Ø       DO 23 I=1,2Ø
-7152    23 P(I)=X(8,I)
-7284       DO 99 I=1,9
-7296       DO 99 J=1,23
-73Ø8    99 X(I,J)=Ø.
-7452  C    GENERATE N MATRIX
-7452       DO 3 I=1,9
-7464     3 X(I,1)=R(I,1)
-7572       DO 4 J=2,1Ø
-7584     4 X(1,J)=R(1,J)/X(1,1)
-7752       DO 5 I=2,9
-7764     5 X(I,2)=R(I,2)-X(I,2)*X(I,1)
-7932       DO 55 J=3,1Ø
-7944    55 X(2,J)=(R(2,J)-X(1,J)*X(2,1))/X(2,2)
-8196       DO 44 I=2,9
-82Ø8       IK=I-1
-8244       DO 33 J=I,9
-8256       X(J,I)=R(J,I)
-84ØØ       DO 33 K=1,IK
-8412    33 X(J,I)=X(J,I)-X(K,I)*X(J,K)
-8784       IF (X(I,I)) 34,56,34
-89ØØ    56 X(I,I)=1.
-8972    34 IM=I+1
-9ØØ8       DO 35 J=IM,1Ø
-9Ø2Ø       X(I,J)=R(I,J)/X(I,I)
-9236       DO 35 K=1,IK
-9248    35 X(I,J)=X(I,J)-X(K,J)*X(I,K)/X(I,I)
-9692    44 CONTINUE
-9728  C    COMPUTE DELTA LOG T AND DELTA LOG P14-P2Ø
-9728       V(1)=X(9,1Ø)
-974Ø       DO 6 J=2,9
-9752       K=1Ø-J
-9788       L=J-1
-9824       V(J)=X(K,1Ø)
-9896       DO 6 I=1,L
-99Ø8       IM=1Ø-I
-9944     6 V(J)=V(J)-X(K,IM)*V(I)
J02Ø8  C    COMPUTE DELTA LOG P(I) AND STORE IN ROW 9 OF X-MATRIX
JØ2Ø8       DO 1Ø J=1,2Ø
JØ22Ø       X(9,J)=Y(9,J)*V(1)-Y(1Ø,J)
JØ412       DO 1Ø I=1,7
JØ424       K=1Ø-I
JØ46Ø    1Ø X(9,J)=X(9,J)+Y(I,J)*V(K)
JØ76Ø  C    COMPUTE DELTA LOG P(N+1) STORE IN ROW 9 OF Y-MATRIX
JØ76Ø       L=M
JØ772       M=M+13
JØ8Ø8       DO 11 I=1,N
JØ82Ø    11 Y(9,I)=LOG(P(I))*.434294+X(9,I)
```

```
J1024        DO 12 I=14,M
J1036     12 Y(9,I)=LOG(P(I))*.434294+X(9,I)
J1240  C     COMPUTE DELTA LOG A(N+1),T(N+1)
J1240        A(1)=LOG(A(1))*.434294+V(2)
J1288        T(1)=LOG(T(1))*.434294+V(1)
J1336        T(1)=EXP(T(1)/.434294)
J1384        A(1)=EXP(A(1)/.434294)
J1432        PUNCH 102,T(1)
J1456        LL=101
J1468        PUNCH 200,N,L,LL
J1516        LL=201
J1528        PUNCH 100,A(1),C(1),T(1),LL
J1588        DO 7 I=1,N
J1600        LL=300+I
J1636      7 PUNCH 101,Y(9,I),LL
J1756        DO 8 I=14,M
J1768        LL=300+I
J1804      8 PUNCH 101,Y(9,I),LL
J1924        STOP
J1936    200 FORMAT (I3,I2,71X,I4)
J1976    100 FORMAT (3E14.6,34X,I4)
J2020    101 FORMAT (E14.6,62X,I4)
J2054    102 FORMAT (F8.2)
J2076        END
T9999 SIN
T9989 SINF
T9979 COS
T9969 COSF
T9959 EXP
T9949 EXPF
T9939 LOG
T9929 LOGF
T9919 SQRT
```



```
T9909 SQRTF
T9899 ABS
T9889 ABSF
T9879 DRH
T9869 DRHF
T9859 ATAN
T9849 ATANF
T9839 X     T7779
T7769 Y     T5479
T5469 A     T5469
T5459 C     T5459
T5449 T     T5449
T5439 R     T4549
T4539 P     T4349
T4339 V     T4259
T4249 0200
T4239 N
T4229 M
T4219 0022
T4209 I
T4199 K
T4189 0000000000
T4179 J
T4169 000
T4159 0023
T4149 0099
T4139 0003
T4129 0004
T4119 0005
T4109 0055
T4099 001
T4089 0044
T4079 IK
```

T4069 ØØØ1
T4059 ØØ33
T4049 ØØ34
T4039 ØØ56
T4029 5110000000
T4019 1M
T4009 ØØ35
T3999 ØØØ6
T3989 ØØ10
T3979 L
T3969 ØØ1Ø
T3959 ØØ13
T3949 ØØ11
T3939 5Ø43429400
T3929 ØØ12
T3919 Ø1Ø2
T3909 LL
T3899 Ø1Ø1
T3889 Ø2Ø1
T3879 Ø1ØØ
T3869 ØØØ7
T3859 Ø300
T3849 Ø1Ø1
T3839 ØØØ8

LOAD SUBROUTINES
PDQ FIXED FMT SUBROUTNS 11/63
PROCESSING COMPLETE

DATA CARD LAYOUT FORMS

JOB Input FORMAT (THERMO. FUNCT) DEPT. RESEARCH DATA CARD LAYOUT DATE 10-5-65

TEMP. CARD

XXXXXXXX.X

TABLE I

α	B*10³	γ*10⁶	δ*10⁹	C	K	ID
±XX.XXX	XXX±XXX.XXXX	X±XX.XXXXX	±XXX.XXXXX	±XXX.XXXXX	X±XX.XXXXXX	XXX

1

TABLE II

a	b*10³	c*10⁶	δ*10⁹	m
±XX.XX	XXX±XXX.XXXX	X±XX.XXXXX	±XXX.XXXXX	±XXX.XXXXXX

2

TABLE III

A	B*10³	C*10⁶	Δ*10⁹	L	M
±XX.XX	XXX±XXX.XXXX	X±XX.XXXXX	±XXX.XXXXX	±XXX.XXXXX	X±XX.XXXXX

3

JOB OUTPUT FORMAT (THERMO. FUNCT) DEPT. RESEARCH DATA CARD LAYOUT DATE 10-5-65 PAGE ____ OF ____

C_p^o		H_T^o		$\Delta H/RT$		LOG K		S_T^o							ID
±XXX.	XXXX	±XXX.X	XXX	±XXX.X	XXX	±XXX.X	XXX	±XXX	.XXXX						X4XX

ENGINEERING COMPUTER APPLICATIONS GROUP

7.4.2

JOB Input Format (Comb. Proc. I) DEPT. RESEARCH DATA CARD LAYOUT DATE 10-6-65 PAGE 1 OF 1

Card	Columns 1–80 (field layout)	Card no.
1	N M: XXXXXX	1.01
2	XX.XX A: XXXE+05 XXX.XXXX P: XXXE+07 XXX.XXX T: XXXE+07	2.01
3	±XX.X LOG P_1: XXXXE+00	3.01
3	±XX.X LOG P_2: XXXXE+00	3.02
⋮		⋮
4	±XXX. C_P^0: XXXX ±XXX.X H_T^0: XXX ±XXX.XXXX ΔH/RT: ±XXX.XXX LOG K_1: X ±XXX.XXXX S_T^0	4.01
4	±XXX.XXXX ±XXX.XXXX ±XXX.XXXX ±XXX.XXXX ±XXX.XXXX	4.02
⋮		⋮
5	±XXX. a_0: XXXX ±XXX. b_0: XXXX ±XXX. c_0: XXXX ±XXX. d_0: XXXX ±XXX. e_0: XXXX ±XXX. f_0: XXXX ±XXX. g_0: XXXX ±XXX. h_0: XXXX	5.01
6	±XXX. a_1: XXXX ±XXX. b_1: XXXX ±XXX. c_1: XXXX ±XXX. d_1: XXXX ±XXX. e_1: XXXX ±XXX. f_1: XXXX ±XXX. g_1: XXXX	6.01
6	±XXX. a_2: XXXX ±XXX. b_2: XXXX ±XXX. c_2: XXXX ±XXX. d_2: XXXX ±XXX. e_2: XXXX ±XXX. f_2: XXXX ±XXX. g_2: XXXX	6.02
⋮		⋮

ENGINEERING COMPUTER APPLICATIONS GROUP

JOB Comb. Process II (output) DEPT. RESEARCH DATA CARD LAYOUT DATE 11-2-65 PAGE 1 OF 1

XXXXX.XX TEMPERATURE CARD

XXXXXX 101

No. OF COMPOUNDS — No. OF ELEMENTS

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX 201

A P T

XXXXXXXXXXXXXXX 301

XXXXXXXXXXXXXXX 302

P(i)

ENGINEERING COMPUTER APPLICATIONS GROUP

Block Diagrams

IBM DIAGRAMMING AND CHARTING WORKSHEET

Application COMBUSTION PROCESS

Procedure THERMODYNAMIC FUNCTIONS

Date 10-5-65

Drawn By YM & M

Page 1 of 1

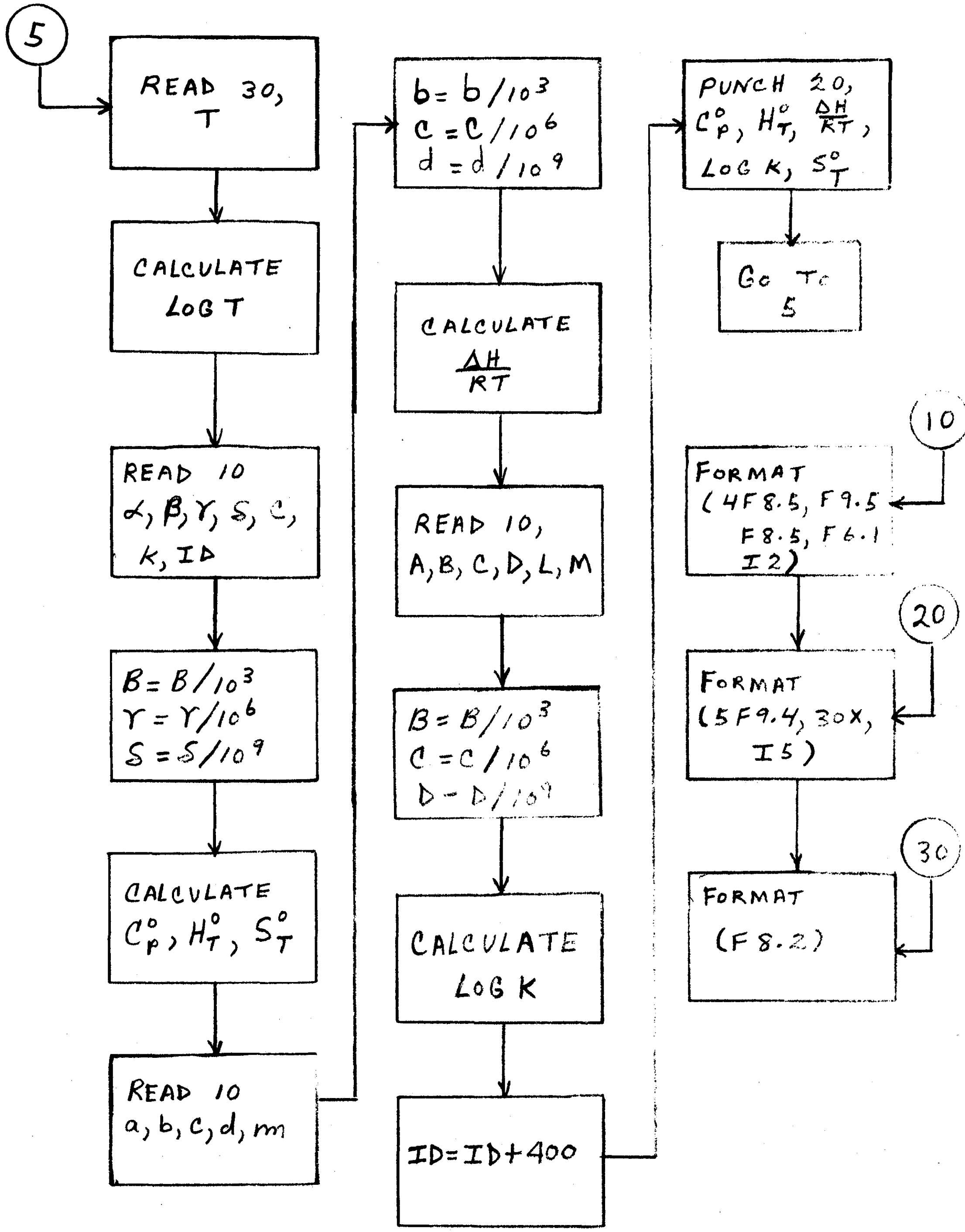


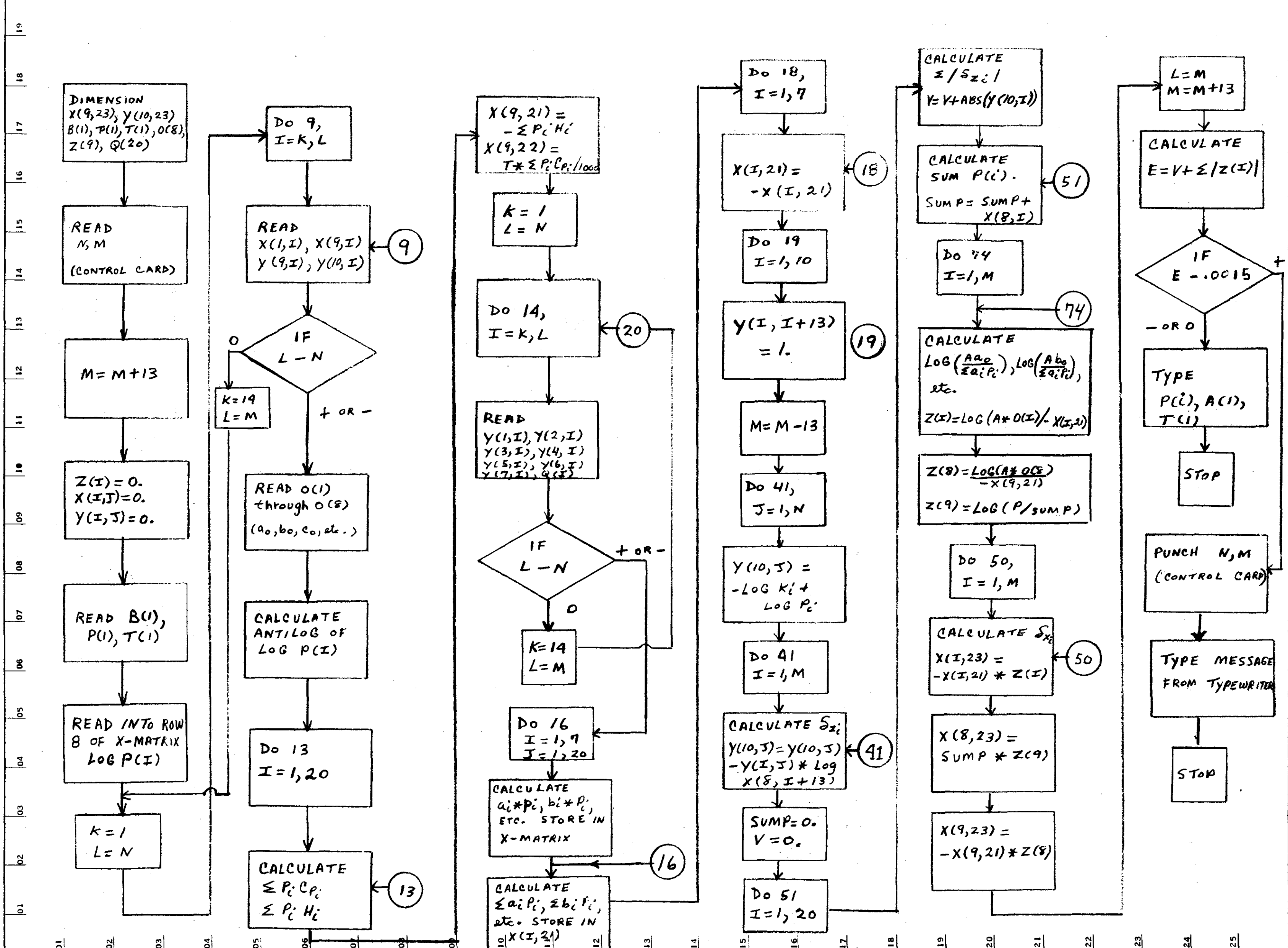
DIAGRAM OF THERMODYNAMIC FUNCTIONS PROGRAM

Fold under at dotted line.

IBM DIAGRAMMING AND CHARTING WORKSHEET

Application COMBUSTION PROCESS I   Date 10-6-65   Page 1 of 1

Procedure   Drawn By MEM



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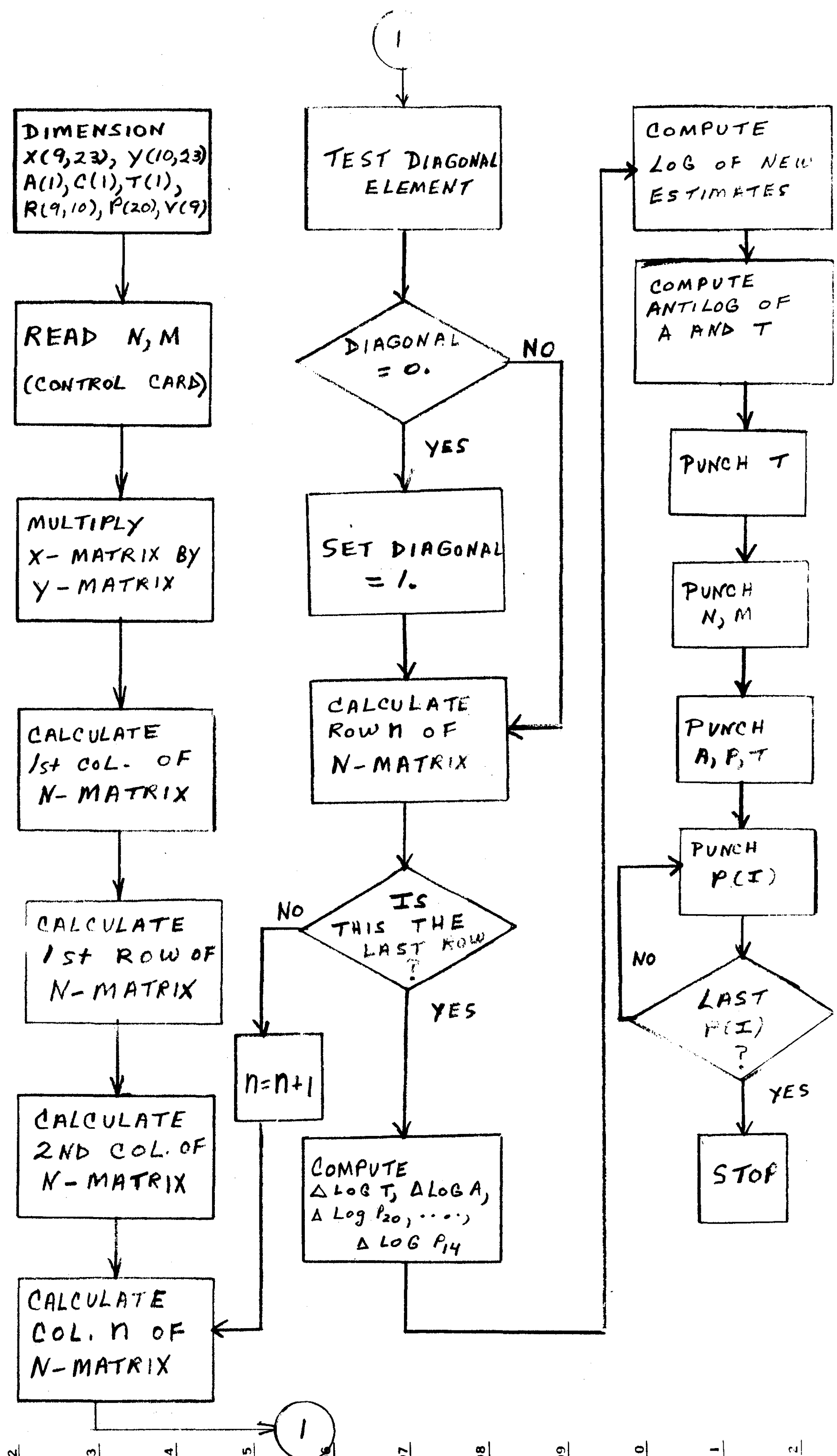
IBM DIAGRAMMING AND CHARTING WORKSHEET

Application COMBUSTION PROCESS II   Date 10-7-65   Page 1 of 1

Procedure   Drawn By MEM



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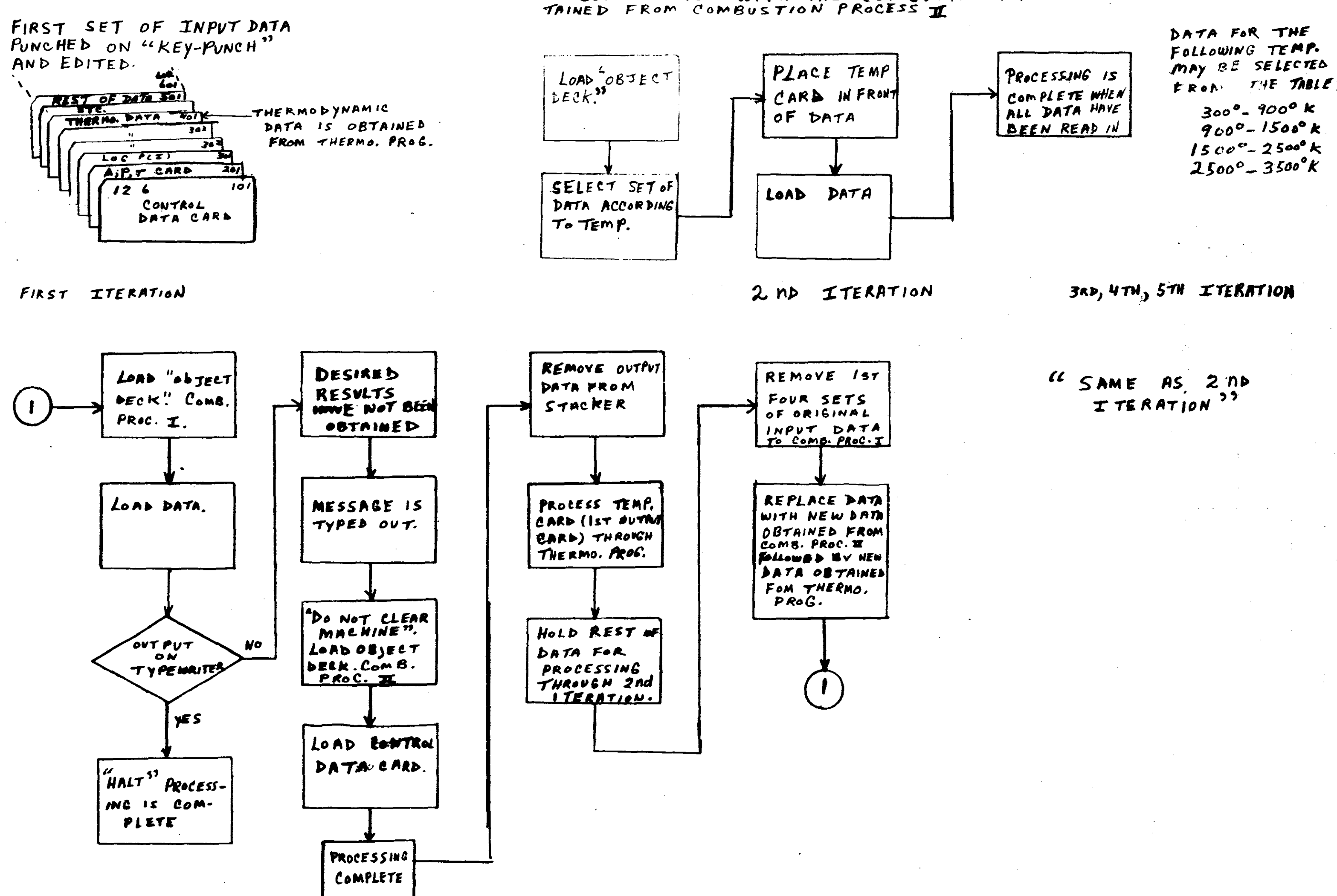
IBM DIAGRAMMING AND CHARTING WORKSHEET

Application Comb. Process I, Comb. Process II, & Thermody. Funct. Date 11-3-65 Page 1 of 1

Procedure Operating Procedure Drawn By

THERMODYNAMIC FUNCTIONS PROGRAM

1ST TEMP. CARD WILL BE PUNCHED ON "KEY-PUNCH." ALL OTHER USED IN CONJUNCTION WITH THE COMBUSTION PROCESS PROGRAM WILL BE OBTAINED FROM COMBUSTION PROCESS II



Fold under at dotted line.

COEFFICIENTS OF THERMODYNAMIC DATA TABLES

TABLE II

Coefficients and Constants for C_p, H_T, and S_T Equations

	Temp. °K	α	$\beta \times 10^3$	$\gamma \times 10^6$	$\delta \times 10^9$	C	k
Argon							
	300-900	4.96810	0.00000	0.00000	0.00000	0.00000	8.67690
	900-1500	4.96810	0.00000	0.00000	0.00000	0.00000	8.67698
	1500-2500	4.96810	0.00000	0.00000	0.00000	0.00000	8.67698
	2500-3500	4.96810	0.00000	0.00000	0.00000	0.00000	8.67701
Br (gas)							
	300-900	4.97787	- 0.01110	- 0.16179	0.31111	26.55610	13.45102
	900-1500	5.06468	- 0.67585	1.02643	-0.30833	26.56008	13.12811
	1500-2500	3.94566	1.64307	- 0.58561	0.06731	26.96793	19.22429
	2500-3500		No data presently available				
Br_2 (gas)							
	300-900	7.56238	5.23254	- 6.79762	3.05556	7.56818	14.27127
	900-1500	8.32286	1.46984	- 1.05952	0.27778	7.46947	10.83361
	1500-2500	8.08510	1.38077	- 0.63636	0.10490	7.66888	12.43490
	2500-3500		No data presently available				
C (graphite)							
	300-900	-1.37805	14.37016	-10.56905	2.72222	92.03903	5.38493
	900-1500	1.78343	5.76758	- 3.01310	0.61111	91.18775	-10.92577
	1500-2500	3.69097	2.06002	- 0.55082	0.05206	90.43503	-21.45576
	2500-3500	5.26020	0.45665	- 0.01772	-0.00505	89.30364	-31.09357
C (gas)							
	300-900	5.01446	- 0.17263	0.22869	-0.10278	261.99066	9.23312
	900-1500	4.94401	0.08499	- 0.09298	0.03333	262.00556	9.57770
	1500-2500	5.15597	- 0.28602	0.12290	-0.00845	261.91504	8.38824
	2500-3500	5.24324	- 0.43913	0.20430	-0.02211	261.88475	7.90497

TABLE II (continued)

Temp. °K	α	$\beta \times 10^3$	$\gamma \times 10^6$	$\delta \times 10^9$	C	k
CO (gas)						
300-900	7.40128	- 3.29913	7.16238	-3.35833	65.70215	5.74348
900-1500	5.36912	4.06773	- 1.80345	0.29722	66.12654	15.67967
1500-2500	6.20126	2.55577	- 0.88801	0.11249	65.78319	11.03990
2500-3500	7.43752	1.00433	- 0.23500	0.02038	65.03924	3.68506
CO_2 (gas)						
300-900	4.62716	18.19396	-14.66429	4.86389	0.17012	19.89164
900-1500	6.57128	11.09794	- 5.82321	1.13611	- 0.24259	10.37873
1500-2500	9.63218	5.02247	- 1.76740	0.22673	- 1.41059	- 6.43266
2500-3500	12.11555	1.88641	- 0.43936	0.03831	- 2.89546	-21.19119
COS (gas)						
300-900	5.03988	22.22610	-22.13774	8.58889	159.12375	20.89278
900-1500	8.33898	9.27936	- 5.00821	1.00556	158.48017	5.00947
1500-2500	11.08096	3.79860	- 1.32033	0.17053	157.44110	-10.03149
2500-3500	12.94778	1.43330	- 0.31585	0.02768	156.32907	-21.11925
CS_2 (gas)						
300-900	6.34585	20.63475	-20.53964	7.70000	317.51697	15.36936
900-1500	9.82266	7.84001	- 4.55571	0.96111	316.79158	- 1.60107
1500-2500	12.43216	2.51804	- 0.90414	0.11890	315.82254	-15.86241
2500-3500	13.72348	0.86699	- 0.19699	0.01754	315.06061	-23.52007
H (gas)						
300-900	4.96810	0.00000	0.00000	0.00000	85.33693	- 0.91384
900-1500	4.96810	0.00000	0.00000	0.00000	85.33691	- 0.91379
1500-2500	4.96810	0.00000	0.00000	0.00000	85.33690	- 0.91377
2500-3500	4.96810	0.00000	0.00000	0.00000	85.33690	- 0.91376
H_2 (gas)						
300-900	6.34442	3.06954	- 4.90655	2.76111	67.45133	- 5.65734
900-1500	7.62194	- 2.25177	2.45762	-0.60833	67.22029	-11.72213
1500-2500	5.80531	1.47043	- 0.10349	-0.01733	67.68494	- 1.80405
2500-3500	5.87503	1.69951	- 0.32162	0.02894	67.68494	- 2.48129

TABLE II (continued)

Temp. °K	α	$\beta \times 10^3$	$\gamma \times 10^6$	$\delta \times 10^9$	c	k
HBr (gas)						
300-900	7.40347	- 2.78673	5.03202	-1.92778	25.26861	5.90995
900-1500	4.82434	4.71588	- 2.25298	0.43889	25.93819	19.08726
1500-2500	5.64971	2.93791	- 0.95458	0.11886	25.64684	14.61765
2500-3500		No data presently available				
H_2O (gas)						
300-900	7.96504	- 1.18130	5.26881	-2.22222	11.33351	- 0.13970
900-1500	7.16810	1.74167	1.53476	-0.58611	11.50568	3.76506
1500-2500	4.95233	6.38682	- 1.72814	0.18124	12.30309	15.80923
2500-3500	6.62109	4.43561	- 0.96469	0.08125	11.22879	5.76574
H_2S (gas)						
300-900	7.69475	- 0.00779	6.45881	-3.18056	162.27594	5.06417
900-1500	5.19272	8.32854	- 2.89714	0.35556	162.84491	17.51098
1500-2500	6.06270	7.02346	- 2.30861	0.28578	162.43440	12.52268
2500-3500	9.11515	3.21967	- 0.71886	0.06309	160.58488	- 5.65846
N (gas)						
300-900	4.96810	0.00000	0.00000	0.00000	113.42918	8.30830
900-1500	4.97213	- 0.01102	0.00976	-0.00278	113.42811	8.28757
1500-2500	4.89391	0.13226	- 0.07869	0.01568	113.46040	8.72343
2500-3500	4.91189	0.14696	- 0.09934	0.02044	113.43050	8.58571
N_2 (gas)						
300-900	7.38656	- 2.98433	6.01631	-2.61111	1.65402	4.33152
900-1500	5.49194	3.44012	- 1.28357	0.16667	2.07553	13.71896
1500-2500	5.95705	2.71090	- 0.92791	0.11599	1.86228	11.06826
2500-3500	7.20928	1.14339	- 0.26995	0.02345	1.10708	3.61543
NO (gas)						
300-900	7.83854	- 5.03549	10.46357	-5.20833	23.34538	6.76643
900-1500	5.46742	4.48819	- 2.25417	0.42222	23.78872	18.10630
1500-2500	6.64779	2.21014	- 0.77591	0.09955	23.32637	11.59108
2500-3500	7.74594	0.82499	- 0.19014	0.01657	22.66911	5.06361

TABLE II (continued)

Temp. °K	α	$\beta \times 10^3$	$\gamma \times 10^6$	$\delta \times 10^9$	C	k
NO_2 (gas)						
300-900	6.07017	10.18474	- 2.27786	-1.43611	11.76362	19.83972
900-1500	6.43739	11.25150	- 6.39881	1.33056	11.54805	17.37746
1500-2500	10.10326	3.84337	- 1.35869	0.17694	10.17349	- 2.69188
2500-3500	12.06415	1.35745	- 0.30247	0.02667	9.00610	-14.33726
O (gas)						
300-900	5.82447	- 2.93332	3.68702	-1.60000	59.97630	6.00725
900-1500	5.18254	- 0.35423	0.21798	-0.04722	60.09763	9.08008
1500-2500	5.01322	- 0.01167	- 0.01484	0.00591	60.16089	10.00671
2500-3500	5.15709	- 0.17073	0.04354	-0.00120	60.06363	9.13323
O_2 (gas)						
300-900	6.86954	- 0.97686	6.00619	-3.63056	2.05967	9.92168
900-1500	5.64527	4.87180	- 2.79798	0.61667	2.23511	15.51879
1500-2500	7.61206	0.94407	- 0.16012	0.02108	1.48991	4.72934
2500-3500	7.82021	0.58387	0.03146	-0.01127	1.41325	3.57106
OH (gas)						
300-900	7.58972	- 2.19358	2.50464	-0.56667	43.90179	1.19689
900-1500	7.20029	- 1.33427	2.02286	-0.55833	44.01996	3.26569
1500-2500	5.38982	2.43528	- 0.61041	0.05829	44.67687	13.12034
2500-3500	5.89037	1.88039	- 0.40655	0.03351	44.33976	10.08323
S (gas)						
300-900	6.01259	- 1.11469	- 0.39298	0.65833	164.70040	6.17447
900-1500	5.90721	- 1.39923	0.77048	-0.14167	164.75922	6.87100
1500-2500	5.71818	- 0.94930	0.41903	-0.05130	164.81760	7.87223
2500-3500	5.20717	- 0.37068	0.20042	-0.02374	165.15635	10.96340
S_2 (gas)						
300-900	5.70207	9.85685	-11.24595	4.56944	228.79248	19.54349
900-1500	7.77137	2.00324	- 1.20259	0.26389	228.37683	9.51470
1500-2500	8.48089	0.53176	- 0.17635	0.02345	228.11776	5.64902
2500-3500	8.72567	0.21443	- 0.03888	0.00355	227.97571	4.20115

TABLE II (continued)

	Temp. °K	α	$\beta \times 10^3$	$\gamma \times 10^6$	$\delta \times 10^9$	C	k
SO_2 (gas)	300-900	5.95304	14.68612	- 9.71143	2.04722	30.81721	21.41043
	900-1500	7.92609	9.42242	- 5.50357	1.16944	30.29440	11.23559
	1500-2500	11.10546	2.92319	- 1.03367	0.13607	29.11630	- 6.13302
	2500-3500	12.59610	1.01911	- 0.21895	0.01941	28.23600	-14.97395
SO_3 (gas)	300-900	4.53177	33.15342	-28.72571	9.21944	9.10707	26.83475
	900-1500	9.87962	15.56309	- 9.25952	1.97222	7.87669	0.16531
	1500-2500	15.23516	4.60266	- 1.71284	0.22566	5.89454	-29.08528
	2500-3500	17.71931	1.43245	- 0.35721	0.03160	4.42565	-43.82149

TABLE III

Coefficients and Constants for $-\Delta H/RT$ Equations

Temp. °K	a	$b \times 10^3$	$c \times 10^6$	$d \times 10^9$	m
Br_2 (gas)					
300-900	1.20436	- 1.32211	1.08593	-0.30612	22.91800
900-1500	0.90905	- 0.70996	0.52206	-0.11252	22.97167
1500-2500	-0.09751	0.47940	-0.08971	0.00374	23.28180
2500-3500		No data presently available			
CO (gas)					
300-900	1.72984	0.04861	-0.54458	0.20827	128.95384
900-1500	2.39396	- 1.09122	0.32347	-0.03914	128.80884
1500-2500	1.99668	- 0.71794	0.16708	-0.01447	128.96790
2500-3500	1.49090	- 0.40613	0.08099	-0.00550	129.27807
CO_2 (gas)					
300-900	6.05670	- 6.09715	3.73496	-1.02738	192.11031
900-1500	4.39692	- 2.94914	1.03429	-0.15061	192.44760
1500-2500	2.79290	- 1.34150	0.31209	-0.02810	193.05350
2500-3500	1.73197	- 0.67102	0.12157	-0.00790	193.68752
COS (gas)					
300-900	5.94368	- 6.65407	4.30416	-1.21189	164.82172
900-1500	3.87205	- 2.75450	0.99026	-0.14607	165.24372
1500-2500	2.41861	- 1.26948	0.30988	-0.02823	165.78225
2500-3500	1.33834	- 0.60733	0.12817	-0.00940	166.44810
CS_2 (gas)					
300-900	5.38117	- 5.79611	3.35175	-0.81596	137.81513
900-1500	3.49011	- 2.65528	1.00703	-0.15236	138.24684
1500-2500	2.09342	- 1.18320	0.31284	-0.02893	138.74767
2500-3500	0.97325	- 0.51515	0.13455	-0.01096	139.45676

TABLE III (continued)

	Temp. °K	a	$b \times 10^3$	$c \times 10^6$	$d \times 10^9$	m
H_2 (gas)						
	300-900	1.80740	- 0.77231	0.82300	-0.34735	51.94214
	900-1500	1.16455	0.56655	-0.41223	0.07653	52.05838
	1500-2500	2.07869	- 0.36996	0.01736	0.00218	51.72101
	2500-3500	2.04360	- 0.42760	0.05395	-0.00364	51.82455
HBr (gas)						
	300-900	1.27940	0.69836	-0.87118	0.28166	43.58988
	900-1500	2.62092	- 1.35657	0.55007	-0.09400	43.25493
	1500-2500	1.64249	- 0.32578	0.06189	-0.00649	43.60677
	2500-3500	No data presently available				
H_2O (gas)						
	300-900	3.92280	- 0.44081	-0.26532	0.07828	110.36133
	900-1500	4.00080	- 0.52733	-0.22087	0.06779	110.33572
	1500-2500	5.03059	- 1.60988	0.28738	-0.02206	109.96629
	2500-3500	4.26326	- 1.15897	0.16912	-0.01037	110.45794
H_2S (gas)						
	300-900	4.15348	- 0.27850	-1.14929	0.48294	87.10401
	900-1500	5.35948	- 2.44753	0.61519	-0.06255	86.84728
	1500-2500	4.82659	- 2.00597	0.45752	-0.04241	87.08322
	2500-3500	3.03344	- 0.90334	0.15420	-0.01092	88.18437
N_2 (gas)						
	300-900	1.28299	0.75087	-1.00915	0.32848	113.32404
	900-1500	2.24043	- 0.87109	0.21858	-0.02167	113.11086
	1500-2500	1.92766	- 0.61552	0.12924	-0.01065	113.25067
	2500-3500	1.31563	- 0.21378	0.01196	0.00219	113.60060
NO (gas)						
	300-900	1.48649	0.52891	-1.13667	0.45393	75.51106
	900-1500	2.35865	- 1.22114	0.41630	-0.05941	75.34848
	1500-2500	1.64012	- 0.52574	0.11446	-0.00981	75.62922
	2500-3500	1.16897	- 0.21358	0.02253	0.00033	75.89597

TABLE III (continued)

	Temp. °K	a	b x 10^3	c x 10^6	d x 10^9	m
NO_2 (gas)						
	300-900	5.03724	- 4.03857	1.61896	-0.22190	111.51946
	900-1500	4.47844	- 3.01193	1.14807	-0.17962	111.74950
	1500-2500	2.42399	- 1.87920	0.62917	-0.07520	112.52110
	2500-3500	1.59110	- 0.78095	0.14604	-0.00434	112.99561
O_2 (gas)						
	300-900	2.40502	- 1.23028	0.22944	0.05416	59.32436
	900-1500	2.37503	- 1.40401	0.54244	-0.08946	59.35819
	1500-2500	1.21493	- 0.24340	0.02188	-0.00117	59.79684
	2500-3500	1.25498	- 0.23281	0.00933	0.00111	59.73753
OH (gas)						
	300-900	1.61169	- 0.18612	0.19833	-0.13000	51.03079
	900-1500	1.48464	0.24658	-0.30274	0.06430	51.03237
	1500-2500	2.31047	- 0.61566	0.09990	-0.00659	50.73363
	2500-3500	2.13098	- 0.51607	0.07550	-0.00437	50.85433
S_2 (gas)						
	300-900	3.18182	- 3.04093	1.75451	-0.40920	50.62665
	900-1500	2.03449	- 1.20812	0.46019	-0.06884	50.89501
	1500-2500	1.48721	- 0.61149	0.17015	-0.01596	51.08413
	2500-3500	0.84975	- 0.24048	0.07376	-0.00642	51.49653
SO_2 (gas)						
	300-900	5.89177	- 5.45159	2.79992	-0.57729	127.73154
	900-1500	4.19986	- 2.90101	1.12550	-0.17682	128.14633
	1500-2500	2.33444	- 0.98020	0.23869	-0.02209	128.83220
	2500-3500	1.47201	- 0.43558	0.08495	-0.00573	129.34775
SO_3 (gas)						
	300-900	9.53787	-10.83605	6.60773	-1.68085	168.83660
	900-1500	5.82471	- 4.53514	1.79207	-0.28375	169.66850
	1500-2500	2.77904	- 1.40570	0.35012	-0.03261	170.79080
	2500-3500	1.48906	- 0.58201	0.11545	-0.00742	171.55359

TABLE IV

Coefficients and Constants for Log K Equations

Temp. °K	A	$B \times 10^3$	$\Gamma \times 10^6$	$\Delta \times 10^9$	L	M
Br_2 (gas)						
300-900	-1.20436	0.57418	-0.23581	0.04431	- 2.23727	9.95316
900-1500	-0.90905	0.30833	-0.11336	0.01629	- 2.97500	9.97647
1500-2500	0.09751	-0.20820	0.01948	-0.00054	- 5.72736	10.11116
2500-3500		No data presently available				
CO (gas)						
300-900	-1.72984	-0.02111	0.11825	-0.03015	- 1.32418	56.00394
900-1500	-2.39396	0.47391	-0.07024	0.00567	0.38885	55.94097
1500-2500	-1.99668	0.31180	-0.03628	0.00210	- 0.74022	56.01005
2500-3500	-1.49090	0.17638	-0.01759	0.00080	- 2.27070	56.14475
CO_2 (gas)						
300-900	-6.05670	2.64796	-0.81104	0.14873	2.33406	83.43245
900-1500	-4.39692	1.28079	-0.22459	0.02180	- 1.88410	83.57893
1500-2500	-2.79290	0.58261	-0.06777	0.00407	- 6.39973	83.84207
2500-3500	-1.73197	0.29142	-0.02640	0.00114	- 9.59841	84.11742
COS (gas)						
300-900	-5.94368	2.88983	-0.93464	0.17544	2.46722	71.58117
900-1500	-3.87205	1.19627	-0.21503	0.02115	- 2.80267	71.76444
1500-2500	-2.41861	0.55133	-0.06729	0.00409	- 6.88230	71.99832
2500-3500	-1.33834	0.26376	-0.02783	0.00136	-10.15361	72.28749
CS_2 (gas)						
300-900	-5.38117	2.51722	-0.72782	0.11812	0.97930	59.85235
900-1500	-3.49011	1.15317	-0.21867	0.02206	- 3.93043	60.03984
1500-2500	-2.09342	0.51386	-0.06793	0.00419	- 7.83135	60.25735
2500-3500	-0.97325	0.22373	-0.02922	0.00159	-11.23680	60.56530

TABLE IV (continued)

Temp. °K	A	B x 10^3	Γ x 10^6	Δ x 10^9	L	M
H_2 (gas)						
300-900	-1.80740	0.33541	-0.17871	0.05028	-0.05198	22.55819
900-1500	-1.16455	-0.24605	0.08951	-0.01108	-1.65659	22.60867
1500-2500	-2.07869	0.16067	-0.00377	-0.00032	0.90789	22.46215
2500-3500	-2.04360	0.18570	-0.01171	0.00053	0.74465	22.50712
HBr (gas)						
300-900	-1.27940	-0.30329	0.18918	-0.04077	-0.89267	18.93084
900-1500	-2.62092	0.58915	-0.11945	0.01361	2.64026	18.78538
1500-2500	-1.64249	0.14149	-0.01344	0.00094	-0.09371	18.93818
2500-3500		No data presently available				
H_2O (gas)						
300-900	-3.92280	0.19144	0.05761	-0.01133	0.75972	47.92932
900-1500	-4.00080	0.22902	0.04796	-0.00981	0.97539	47.91820
1500-2500	-5.03059	0.69916	-0.06240	0.00319	3.85222	47.75775
2500-3500	-4.26326	0.50333	-0.03672	0.00150	1.51497	47.97128
H_2S (gas)						
300-900	-4.15348	0.12095	0.24956	-0.06991	1.96065	37.82879
900-1500	-5.35948	1.06295	-0.13359	0.00906	5.05225	37.71730
1500-2500	-4.82659	0.87118	-0.09935	0.00614	3.51185	37.81976
2500-3500	-3.03344	0.39232	-0.03348	0.00158	-1.91574	38.29799
N_2 (gas)						
300-900	-1.28299	-0.32610	0.21913	-0.04755	-2.12757	49.21601
900-1500	-2.24044	0.37831	-0.04746	0.00314	0.34882	49.12342
1500-2500	-1.92766	0.26732	-0.02806	0.00154	-0.55680	49.18414
2500-3500	-1.31563	0.09284	-0.00260	-0.00032	-2.39115	49.33612
NO (gas)						
300-900	-1.48649	-0.22970	0.24682	-0.06571	-1.00421	32.79404
900-1500	-2.35865	0.53033	-0.09040	0.00860	1.18577	32.72343
1500-2500	-1.64012	0.22832	-0.02485	0.00142	-0.84787	32.84535
2500-3500	-1.16897	0.09275	-0.00489	-0.00005	-2.25801	32.96120

TABLE IV (continued)

	Temp. °K	A	B x 10^3	Γ x 10^6	Δ x 10^9	L	M
NO_2 (gas)							
	300-900	-5.30724	1.75393	-0.35155	0.03212	2.19934	48.43229
	900-1500	-4.47844	1.30807	-0.24930	0.02600	- 0.03725	48.53219
	1500-2500	-2.42399	0.81613	-0.13662	0.01089	- 2.49391	48.86729
	2500-3500	-1.59110	0.33916	-0.03171	0.00063	- 6.31454	49.07337
O_2 (gas)							
	300-900	-2.40502	0.53431	-0.04982	-0.00784	0.58712	25.76424
	900-1500	-2.37503	0.60975	-0.11779	0.01295	0.45422	25.77894
	1500-2500	-1.21493	0.10571	-0.00475	0.00017	- 2.81254	25.96944
	2500-3500	-1.25498	0.10111	-0.00203	-0.00017	- 2.66649	25.94368
OH (gas)							
	300-900	-1.61169	0.08083	-0.04307	0.01882	- 0.15157	22.16239
	900-1500	-1.48464	-0.10709	0.06574	-0.00931	- 0.42621	22.16308
	1500-2500	-2.31047	0.26738	-0.02169	0.00095	1.88357	22.03334
	2500-3500	-2.13098	0.22412	-0.01639	0.00063	1.33278	22.08576
S_2 (gas)							
	300-900	-3.18182	1.32066	-0.38099	0.05924	2.95414	21.98688
	900-1500	-2.03449	0.52468	-0.09993	0.00997	- 0.04026	22.10342
	1500-2500	-1.48721	0.26557	-0.03695	0.00230	- 1.56036	22.18556
	2500-3500	-0.84975	0.10444	-0.01602	0.00093	- 3.50471	22.36466
SO_2 (gas)							
	300-900	-5.89177	2.36760	-0.60799	0.08357	3.26278	55.47311
	900-1500	-4.19986	1.25989	-0.24440	0.02560	- 1.19090	55.65325
	1500-2500	-2.33444	0.42570	-0.05183	0.00320	- 6.42058	55.95112
	2500-3500	-1.47201	0.18917	-0.01845	0.00083	- 9.02099	56.17502
SO_3 (gas)							
	300-900	-9.53787	4.70603	-1.43485	0.24333	4.71887	73.32481
	900-1500	-5.82471	1.96959	-0.38914	0.04108	- 4.88888	73.68610
	1500-2500	-2.77904	0.61049	-0.07603	0.00472	-13.43033	74.17350
	2500-3500	-1.48906	0.25276	-0.02507	0.00107	-17.31388	74.50478

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