PREDICTION OF THE PHYSICAL PROPERTIES OF PURE GASES AND LIQUIDS

BY

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ABSTRACT

A computer programmed system for the estimation of physical properties of pure compounds from minimum data input on compound type and structure was developed for both gas and liquid phase conditions.

The properties of the gas phase which can be obtained include:

- gas volume
- compressibility
- normal boiling point
- volume at the normal boiling point
- critical temperature, pressure, volume compressibility
- vapor pressure
- Riedel factor
- acentric factor
- ideal heat capacity
- heat capacity at constant pressure
- heat capacity at constant volume
- dipole moment
- intermolecular distance
- hard sphere volume
- viscosity at low pressure
- viscosity at elevated pressure
- thermal conductivity at low pressure
- thermal conductivity at high pressure
- isothermal enthalpy departure

- isothermal entropy departure
- fugacity coefficient
- heat of vaporization at normal boiling point
- entropy of vaporization at normal boiling point
- heat of formation at stated temperature
- heat of formation for ideal gas at 1 atm and 298°K
- free energy of formation for ideal gas at 1 atm and 298°K

The properties of the liquid phase which can be computed include:

- isothermal enthalpy departure
- isothermal entropy departure
- heat capacity departure
- liquid viscosity
- parachor
- surface tension
- coefficient of thermal expansion
- density

This work expands James P. Haggett's (30) gas physical property program to obtain a more flexible and shorter running program; running time was reduced from 30 minutes as devised by Haggett to a maximum of 8 minutes for this program.

Newly included are:

- a liquid physical property program
- a consolidated data input
- a phase discriminator program

- a reprogrammed gas estimation program
- a program to allow calculation of only specified physical properties from among those in Table IX, page 89
- a program to allow property calculation at various temperature and pressure combinations for one compound without having to input the data deck again.

The minimum input data required are the molecular structure and the temperature and pressure at which the properties are desired. The physical properties program can also use experimentally determined properties if available, with a resulting increase in accuracy of the estimated properties.

If no experimental data input was used, the average error of the gas physical properties was 23.75%; the liquid physical properties, 26.5%. If experimental data is used, the estimated gas physical properties had an average error of 16.99%.

APPROVAL OF THESIS

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INTRODUCTION

Industrial chemical calculations and design problems require physical property data for the considered chemical compounds. Although common gas and liquid properties are tabulated in handbooks, referenced and periodical literature, there are more than 3,000,000 known compounds and 50,000 new compounds are discovered each year (29). Thus, a physical property may not be readily available in the available literature. The physical property must then be estimated or experimentally determined in the laboratory.

In 1969 J.P. Haggett (30) presented a gas physical property estimation program with over thirty estimation methods that combined the accuracy and speed of a computer to get reasonably accurate physical property values. Only the structure and molecular weight of the compound was needed.

The work that is included here expands the above work to obtain a more flexible and shorter running program. Newly included are:

- a liquid physical property program
- a consolidated data input
- a phase discriminator program
- a reprogrammed gas estimation program
- a program to allow calculation of only specified physical properties from among those in the total list
- a program to allow property calculation at various temperature and pressure combinations for one compound without having to input the data deck again.

PROGRAM STRUCTURE

Previous physical property estimation programs were developed by the American Petroleum Industry (API) and the American Institute of Chemical Engineers (AIChE) (40), where both are proprietary systems and not readily available to the chemical engineer. The AIChE program is more recent, and it is similar to this work's program.

The AIChE program requires the input of the boiling point and vapor pressure. If the group structure methods are to be used, the user must input the corresponding numbers himself. Poor estimation performance is obtained for the freezing point, the liquid heat capacity and viscosity. The AIChE program has a driver or executive program to call each method which is programmed as a subroutine for ease of updating. An overall error is obtained for each estimation path and the best result with the least accumulated error is printed out.

For pure organic compounds and mixtures of similar compounds, the AIChE program can estimate engineering properties within what is normally termed engineering accuracy.

In 1969 J.P. Haggett (30) presented a gas physical property estimation program using available estimation methods and recommendations from Reid and Sherwood's The Properties of Gases and Liquids. Unlike the AIChE program, Haggett's included, when recommended, those estimation methods that required an input derived from structure. His overlying theme was to estimate physical properties with only a knowledge of a compound's structure and molecular weight. He then chose the best reccommended estimation technique that aligned with this theme. If that technique had deficiencies in scope (i.e., could not be used for alcohols) he included methods recommended for these deficient areas. Some estimation methods required more data input than just structure (i.e., critical properties, etc.) but these additional inputs could also be estimated from structure.

Each physical property estimation technique was programmed as a subroutine to facilitate instituting estimation improvements. These subroutines were called by an executive program.

Since some physical properties were readily available in the literature, Haggett included an input for the normal boiling point, molar volume at the normal boiling point, critical properties and dipole moment.

The limitations of Haggett's gas physical property estimation program were:

- each estimation technique that required structural input was input separately, increasing the data input requirements;
- every physical property was calculated whether needed or not, increasing running time;
- the input deck had to be input again for each calculation even in only a pressure or temperature change was required; and
- the running time for each complete physical property calculation was thirty-four minutes.

This work uses Haggett's gas physical property estimation program with the additions and modifications listed below:

- a liquid physical property estimation program and a phase discriminator program were added;
- the executive calling program was changed to incorporate both a program to allow calculation of only specified physical properties and also a program to allow property calculations at various temperature and pressure combinations for one compound without having to input the data deck again;
- the structural input was consolidated for eleven of the fourteen methods using them, and the appropriate gas estimation subroutines were reprogrammed to incorporate this change; and
- the executive master overlay program in Haggett's original program was deleted to reduce the running time.

Gas and Liquid Physical Property Estimation Program

Subroutine levels were used as demonstrated by R.C. Norris (1) for an ordered program structure:

Level 0	Level 1	Level 2	Level N
input data	required data from Level 0	required data from Level 1 and possibly from Level 0	required data from Level N-1 and possibly from Levels 1 through N-2

The levels and methods for the gas program were:

Level 0

T,P,WT, experimental values if used
input tables

Level 1

LYDPC (5)	critical pressure via Lyderson's method $Pc = M.W./(\Sigma \text{bond contributions} + .34)^2$ error - 3%*
LYDVC (8)	critical volume via Lyderson's method $Vc = 40 + \Sigma \text{bond contributions}$ error - 2%-3%
OTTB (12)	T_B via Ogata Tsuchida method $T_B = py + q$ p,q - functional group contribution, Table VI, page 76 y - radical type, Table VIII, page 80 compounds with more than a single functional group cannot be calculated error - within 5°K
SVB (14)	Vb via Schroeder's method $Vb = \Sigma \text{bond contributions}$, Table VIII, page 80 error - 2%-3%
BRDCPO (17)	subroutine for Cp° via Bennewitz, Rossner and Dobratz' method see reference for equations cannot be used for triple bonds error - 7%
RDCPO (18)	Cp° via Rihani and Doraiswamy's method $Cp^\circ = a + bT + cT^2 + dT^3$ a,b,c,d - bond contributions, Table VIII, page 80 error - 2%-3%
FHF (20)	heat of formation via Franklin's method $\Delta H^\circ_f = \Sigma \text{bond contributions}$, Table VIII, page 80 halogenated structures cannot be treated error - ±5k cal/g mole
VDHF (20)	heat of formation via Verma and Doraiswamy's method $\Delta H^\circ_f = A + BT$ A,B are based on bond contributions, Table VIII, page 80 esters, anhydrides and conjugated compounds cannot be considered; only chlorine derivatives can be considered

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*errors shown in this listing are errors claimed in the references

BEHF (19)	heat of formation via bond energy method $\Delta H^{\circ}_{f} = \Sigma$ bond contributions from Table VIII page 80 not recommended unless absolutely necessary
GBZC (7)	ZC by additive technique, Garcia-Barcena $ZC = 0.293 - \Sigma$ bond contributions from Table VIII page 80 not applicable to polar or aliphatic halide compounds error - 1%

Level 2

GLZC	Zc via gas law
GLVC	Vc via gas law
EDW (9)	acentric factor via Edmister's method $W = 3/7\ (\theta/[1.-\theta])\ \log Pc - 1.0$ $\theta = Tb/Tc$ error - 5%
MALPHA (10)	Riedel factor by Miller's method $\alpha c = 0.9076\ (1 + [Tbr\ \ln Pc] / [1 - Tbr])$ error - within .1 unit except for phenol and aniline
LYDTC (4)	Tc bia Lyderson's method $Tb/Tc = 0.567 + \Sigma$ bond contributions from Table VIII page 80 error - 2%-5%
BENVB (14)	V_b via Benson's method $Vc/Vb = 0.422 \log Pc + 1.981$ not recommended for nitrites error - 3%
WATTB(11)	Tb via Watson's method $T_b = \theta/Vb^{0.18} \exp(2.77\ Vb^{0.18}/\theta - 2.94)$ $\theta = Tb/Tc$ not recommended for highly polar compounds error - ±15°K
ABWSF (21)	entropy and free energy of formation via Anderson, Beyer and Watson's method see reference for equations bond contributions from Table IV, page 70 error - within 5k cal/g mole
RALPHA (10)	Riedel factor via Riedel's method see reference for equations error - 5%

ALTAL (10)	Riedel factor via alternate method $\alpha c = (W - 0.242)/.203 + 7.0$ W = acentric factor error - same as MALPHA
STLJP (13)	potential parameters by Stiel and Thodos method see reference for equations all critical properties are required
STUOI (23)	low pressure viscosity by Stiel and Thodos method see reference for equations all critical properties are required error - 5%
RPMHS (16)	enthalpy and entropy of vaporization by Riedel-Plank-Miller equation see reference for equations error - 2%
RPMVP (15)	vapor pressure via Riedel-Plank-Miller equation see reference for equations critical properties error - 5%
RKZ (2)	Z,V,H',S' with Redlich-Kwong equation see reference for equation trial and error solution
LYDTB (11)	TB via Lyderson's method $Tb = \theta Tc$ error - within 5 to 10°C

Level 4

TMUO1 (22)	low pressure viscosity by theoretical method see reference for equations for nonpolar gases only error - 2%
DW (9)	acentric factor by definition $w = - \log Pv_{pr}$ (at $Tr = .7$) $- 1.0$
LZC (6)	Zc via Lyderson's method $Zc = 1/(3.43 + [6.7][10^{-9}][\Delta Hvb]^2)$ not recommended for polar compounds error - 3%
CBV (25)	high pressure viscosity via Coremans and Beenakker method see reference for equation for low molecular weight gases

JSTU1 (24)	high pressure viscosity via Jossi, Stiel and Thodos method see reference for equations good for $.1<\rho_r<3$
RKCP (2)	Cp via Redlich- Kwong equation see reference for equations need Tc, Pc, CPO, V

Level 5

RKCV (28)	Cv via Redlich-Kwong equation of state see reference for equation need V, TC, PC, VC, CP

Level 6

BKO (26)	low pressure thermal conductivity via Bromely's method see reference for equations bond contributions from Table VIII page 80 error - 4% nonpolar, 10% polar

Level 7

STK (27)	high pressure thermal conductivity via Stiel and Thodos method see reference for equations error - 20%

The levels and methods for the liquid physical property estimation program were:

Level 0

input data

Level 1

data from the gas program
- critical properties
- Riedel factor
- normal boiling point
- entropy and enthalpy of vaporization at the normal boiling point

Level 2

YWDEN (36) density bia Yen Woods method based on Lyderson, Greenkorn and Hougen tables for pseudo reduced temperatures between .3 and 1.0
not valid for $Tr>1.0$
requires Tc,Pc,Vc,Zc
error - 2%

COTE (33) coefficient of thermal expansion via Smith method
$\beta = .04314/(Tc - T)^{0.641}$
error - 28%

BPARC (31) parachor via McGowan additive method
$P = \Sigma$ bond contributions from Table VIII page 80
error - 8%

Level 3

BVIS (32) viscosity via Thomas method with a known viscosity input
$u = (.1167^{0.5})\ 10^{B}(T - Tr)/Tr$
B is calculated with a known viscosity point at its measurement temperature

BWRCP (39,37) isothermal heat capacity departure via Bennedict, Webb, Rubien equation
see referencefor equations
the B-W-R constants are calculated from the acentric factor correlation of reference 37

ENTYA (38) isothermal enthalpy deviation via Yen Alexander method
analytical equations fitted to the improved Lyderson-Greenkorn-Hougen enthalpy deviation charts
requires Tc,Pc,Vc,Zc
not valid for $Tr>1.0$, $Pr>1.0$, $Pr<.01$, $Tr<.5$

Level 4

SURT (34) surface tension via parachor method
$\sigma = [P(\rho - \rho_v)/M.W.]^{4}$
$\log_{10} \rho_v/\rho_{vb} = 5\ \ T/T_B) - 1.0$
$\rho_{vb} = M.W./(82.06T_B)$
error - 20%

BMRENT (31) isothermal entropy departure via Hirschfelder, Buehler, McGee and Sutton equation of state
requires density, Zc,Pc,Tc,Vc, Riedel factor, isothermal enthalpy departure

The liquid estimation methods - isothermal enthalpy departure, isothermal heat capacity departure, and density - are recommended or valid only for limited ranges of reduced temperature, pressure and density as indicated above in the subroutine level discussion. Extension of a calculation past these limits is printed in the liquid results and for the isothermal heat capacity departure calculation (BWR) equation); the result is also printed.

Whereas the calling and execution of each subroutine is self-explanatory, the data input and how that input is converted for use in the program is not self-explanatory and is described below.

First, each data input is described in the order of machine input (see program printout in the Appendix).

IBCB thru IPARC - These inputs relate which combination of groups in the consolidated input table AADAT (Table VIII, page 80) are used for the appropriate estimation technique. Either the fixed point number 0 (if the group is not used) or 1 (if used) is input in the same group order as listed in AADAT. These data are the same and are input for every estimation.

AMCGC thru Y - Each input is the numberical contribution of a combination of structural groups peculiar to each technique. The group order is the same as the sequential appearance of the pertinent groups (as the order of 1's in IBCB thru IPARC) in AADAT. These data are the same and are input for every estimation.

TC,PC,...FMF,THC,...SURTE,COFTE - Each physical property is set at a value of 0 before every physical property estimation.

APA(N,1),APA(N,2) - This input is used in the program for choosing the calculation of particular physical properties that are listed in APAC (Table IX , page 89). Since a particular property on the APAC list may require the estimation of another property or properties on the list, the input number of all of the newly required properties is input in the order of the desired physical properties as listed in APAC. These data are the same and are input for every estimation.

N - Input of the number of different compounds for which physical properties will be estimated.

New Inputs for Each Compound Tested

NAME - The name of the compound for which physical properties will be estimated.

WT - The molecular weight of the compound.

CCDE (Table III ,page 68) - Considerations that will be input to the executor program to select the correct estimation technique for the compound. If a code is valid for the considered compound, then the index number is input in the allotted data field; if not, then 0 is input.

TC,PC,...DIPOLE - Input of experimental values for these properties. If not known, then 0.0 is read in for that property.

AMCH 3 - Input of the number of CH_3 and CH_2 groups in the compound.

GCGB - Input the index numbers for the pertinent group contributions as listed in Table V, page76.

AMGB - Input the number of times the groups listed in GCGB are present in the compound. These numbers are input on the data card in the same allocated data fields as were the corresponding group index numbers for GCGB.

IKOT - Input the pertinent index number corresponding to the compound structure from Table VI page78.

IYOT - Input the pertinent index number corresponding to the general class of the compound as listed in Table VII page79.

XN, XM, Q - Input the number of atoms in the compound, number of freely rotating bonds in the compound and the number of bonds in the molecule respectively.

GCABW - Input the pertinent index numbers corresponding to the group contributions as listed in Table IV page70.

CALC - Input 1.0 if all physical properties are to be estimated; if only particular properties are to be estimated, and will be input later under APAC, then CALC is 0.0.

ALIQ - Input 1.0 if the compound is in the liquid phase; 0.0

if in the vapor phase, and -1.0 if the phase is not known and the Antoine Cox constants are known and will be input later.

APAC - Input 1.0 if a physical property listed in Table IX, page 89 is to be estimated, 0.0 if not. If CALC is 1.0, this input is all 0.0's.

VISCPTT,TTT - Input a known viscosity and the temperature it was estimated at. Input 0.0's if not known.

SURTPT,TTTT - Input a known surface tension and the temperature is was estimated at. Input 0.0's if not known.

AADAT - Input the index numbers for the pertinent group contributions as listed in Table VIII, page 80.

CADAT - Input the number of times the group as listed in AADAT is present in the compound. This number is input on the data card in the same data field as was the corresponding group index number for AADAT.

PN - Input the number of times the same compound will be run at various temperature and pressure combinations. This will prevent having to input the data deck again.

T,P - Input the temperature and pressure at which the compound's physical properties will be estimated.

The list below shows how the above data inputs are converted and used in the estimation of gas and liquid physical properties.

<u>IBCB thru IPARC</u> - Determine which of the 214 groups listed in AADAT are pertinent to the respective techniques. Below are the relationships between the control variables IBCB thru IPARC, the estimation methods and the input variable used in the subroutine.

Method	Input Variables	Control Variables
LYDTH	GCLYD	IGCLY
LYDPC	GCLYD	IGCLY
LYDVC	GCLYD	IGCLY
SVB	GCS	IGCS
BRDCPO	BCBRD	IBCBR
RDCPO	BCRD	IBCRD
FHF	BCF	IBCF
VDHF	BCVD	IBCVD
BEHF	BCBE	IBCBE
BKO	BCB	IBCB
BPARC	AMCGC	IPARC

<u>The Control Variables</u>: IGCLY thru IPARC listed above are inputs of 214 fixed point 0's and 1's where a 1 indicates that that group which corresponds to that index number in AADAT, is used in the method corresponding to the particular control variable. A zero signifies that the group is not required for that method.

> <u>Example</u>: If the 20th data card field is 1.0 for control variable IBCLY, the group corresponding to index number 20 in AADAT (>NH) is a group used in Lyderson's methods for critical properties.

The control variable input is then collated to the actual input variable GCLYD thru AMCGC which are then used in the appropriate estimation method.

First the AADAT input is converted to a floating point matrix of 214 fields - ADAT where AADAT indicates the index number or field of the functional group and CADAT (the number of times the group is present) is input into that position in the matrix.

> Example: For acetic acid, an AADAT input index number 41 was present one time, as input in CADAT. When the ADAT matrix is formed, the 41st data field is read in at a value equal to CADAT or 1.0. Index numbers not input from AADAT are read into the respective data fields as 0.0.

Finally each of the control variable inputs IGCLY - IPARC is examined and when the data field value is 1, the corresponding field from ADAT is input for the control variable's corresponding input variable (GCLYD - AMCGC). GCLYD - AMCGC have data field sizes equal to the number of 1's in the control variable input and are read in the order of appearance of the 1's in that control input.

> Example: If the 41st data field of IGCLY has a value of 1, then the 41st data field of ADAT, which has a value of 1.0, is input into GCLYD as the 20th data field (IGCLY data field's 1 thru 40 had 19 1's contained within it).

The input variables are then used as both the presence of a pertinent group and the number of times that group is present in the compound.

APAC (Table IX page 89) lists the physical properties that can be estimated without having to estimate the whole physical property package. Each index number is read in in order; and if a property is to be estimated a value of 1.0 is input (otherwise, 0.0). The APA input contains the APAC index numbers of physical properties on the APAC list that must be estimated so the desired property can be estimated.

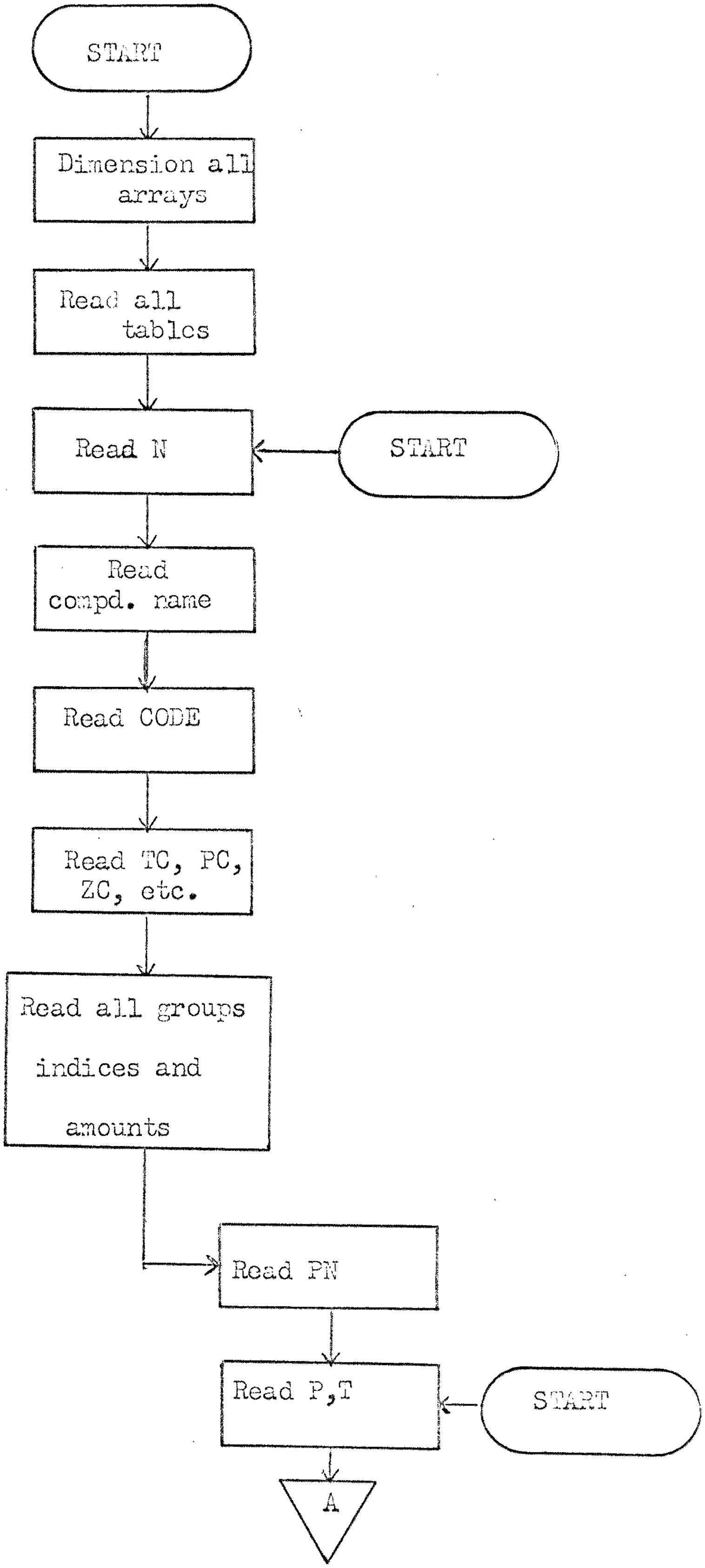
When an APAC data field is 1.0, the corresponding APA index numbers are input to set the required APAC inputs at 1.0 (thus causing the estimation of the required properties).

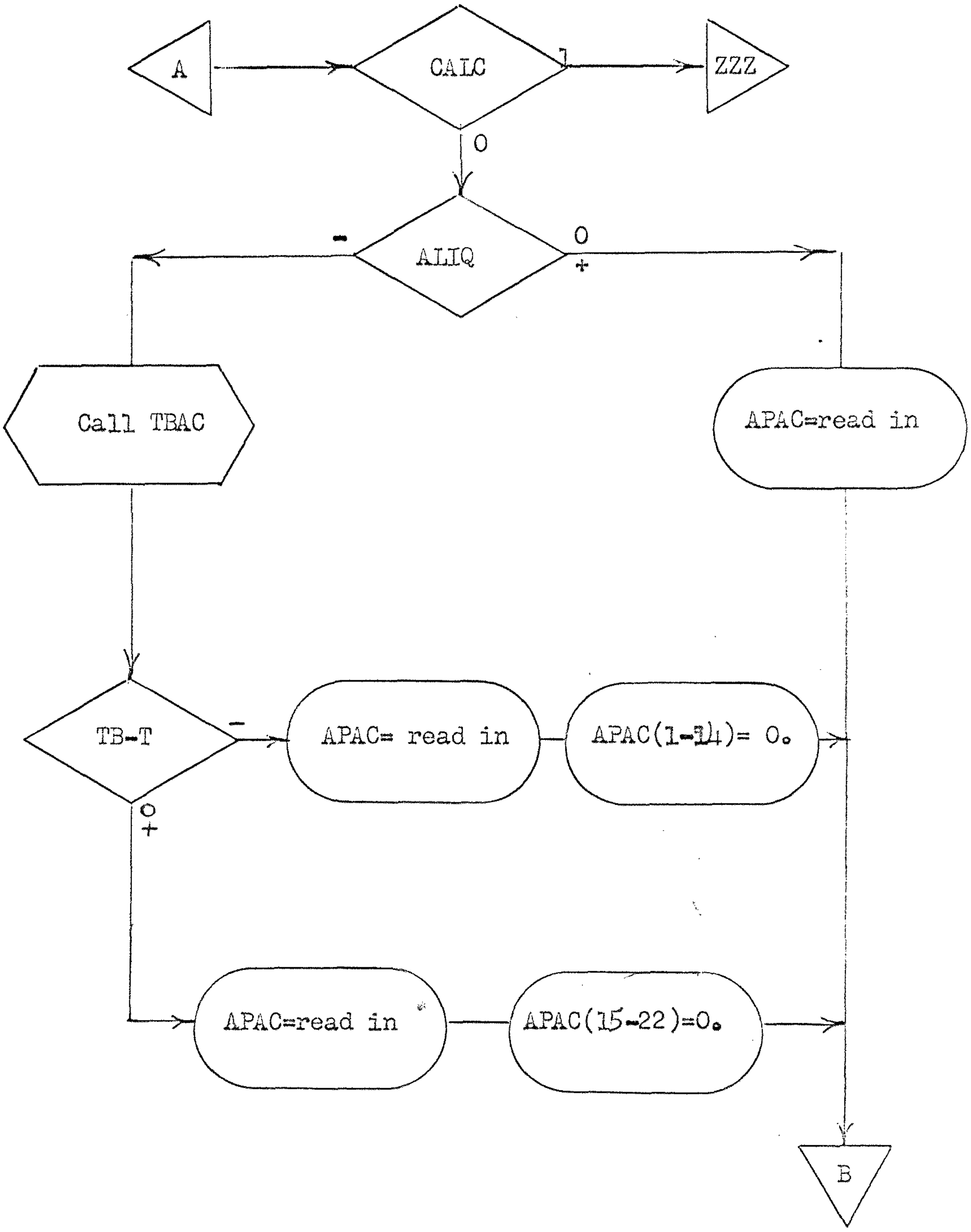
Since there are both liquid and gas physical properties that are chosen by the APAC input, the properties in the phase that is not pertinent are not calculated by setting those APAC data fields at 0.0.

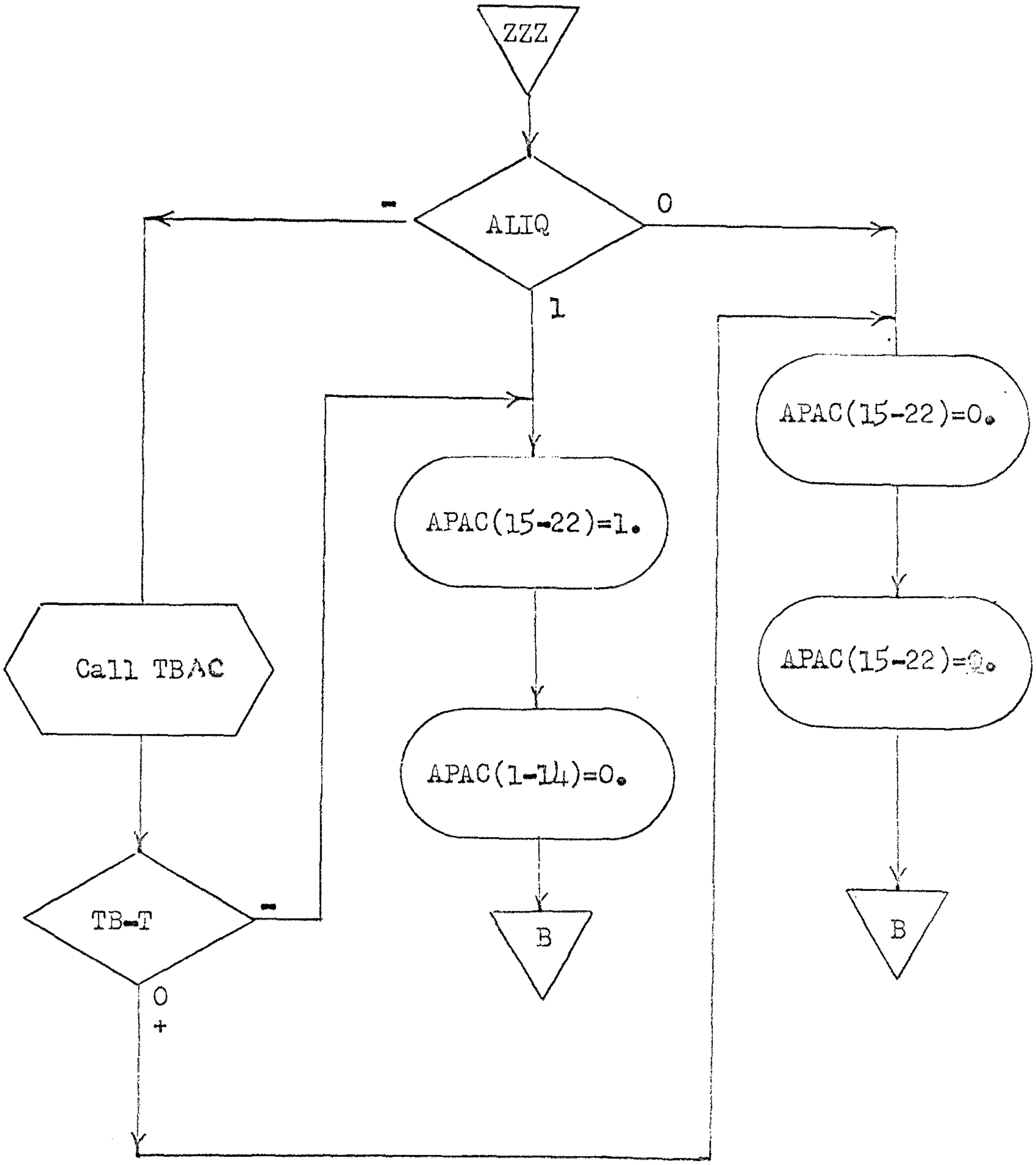
If all the physical properties are to be calculated (CALC=1.0), then, if ALIQ indicated the phase, the other phase is not calculated by setting the appropriate APAC data field at 0.0. The APAC data fields of the wrong phase are also set at 0.0 if ALIQ causes the calculation to estimate the phase with the Antoine Cox equation.

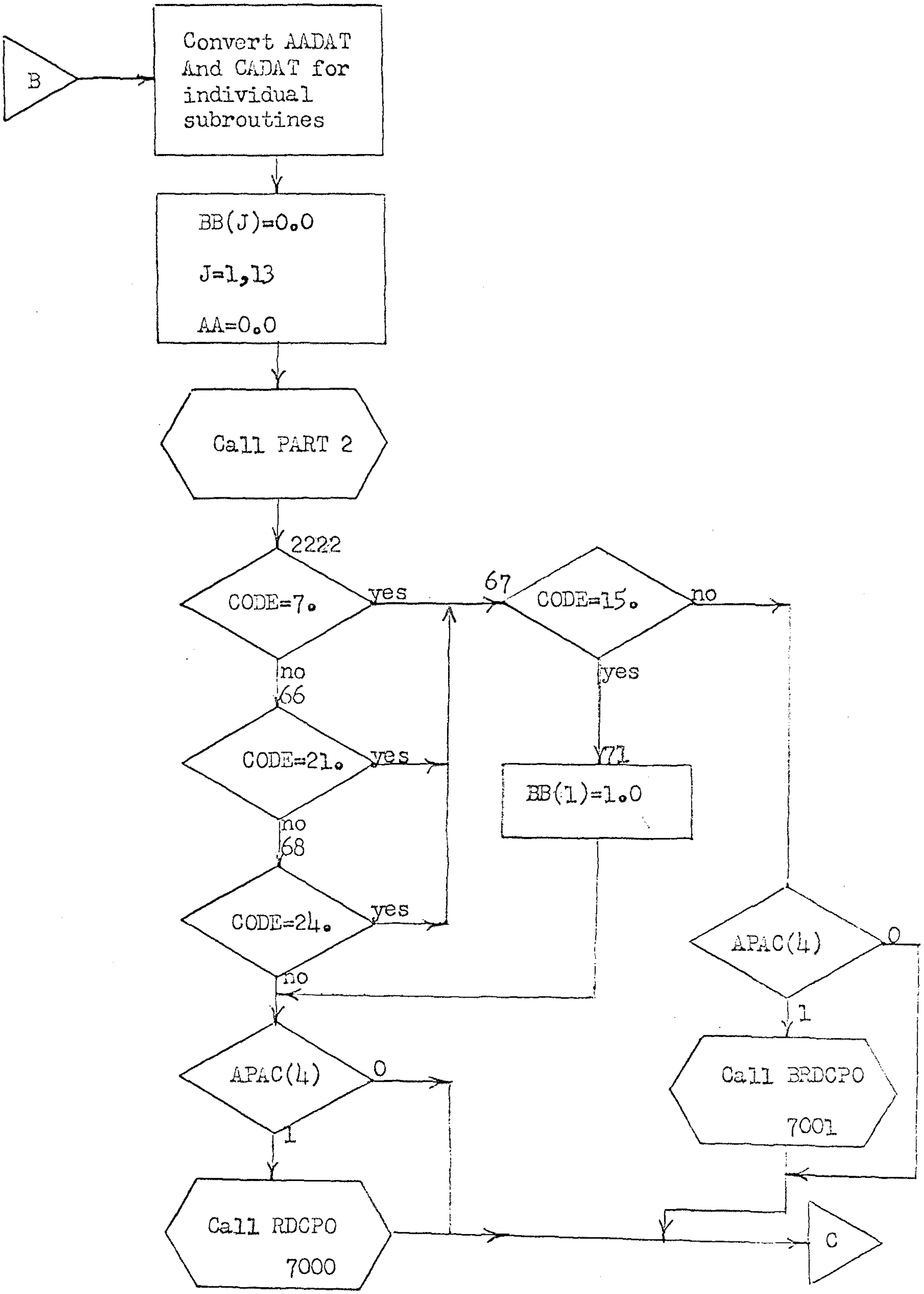
A flow chart is included to assist in following the estimation path through the gas and liquid physical property estimation program. The flow chart is included below.

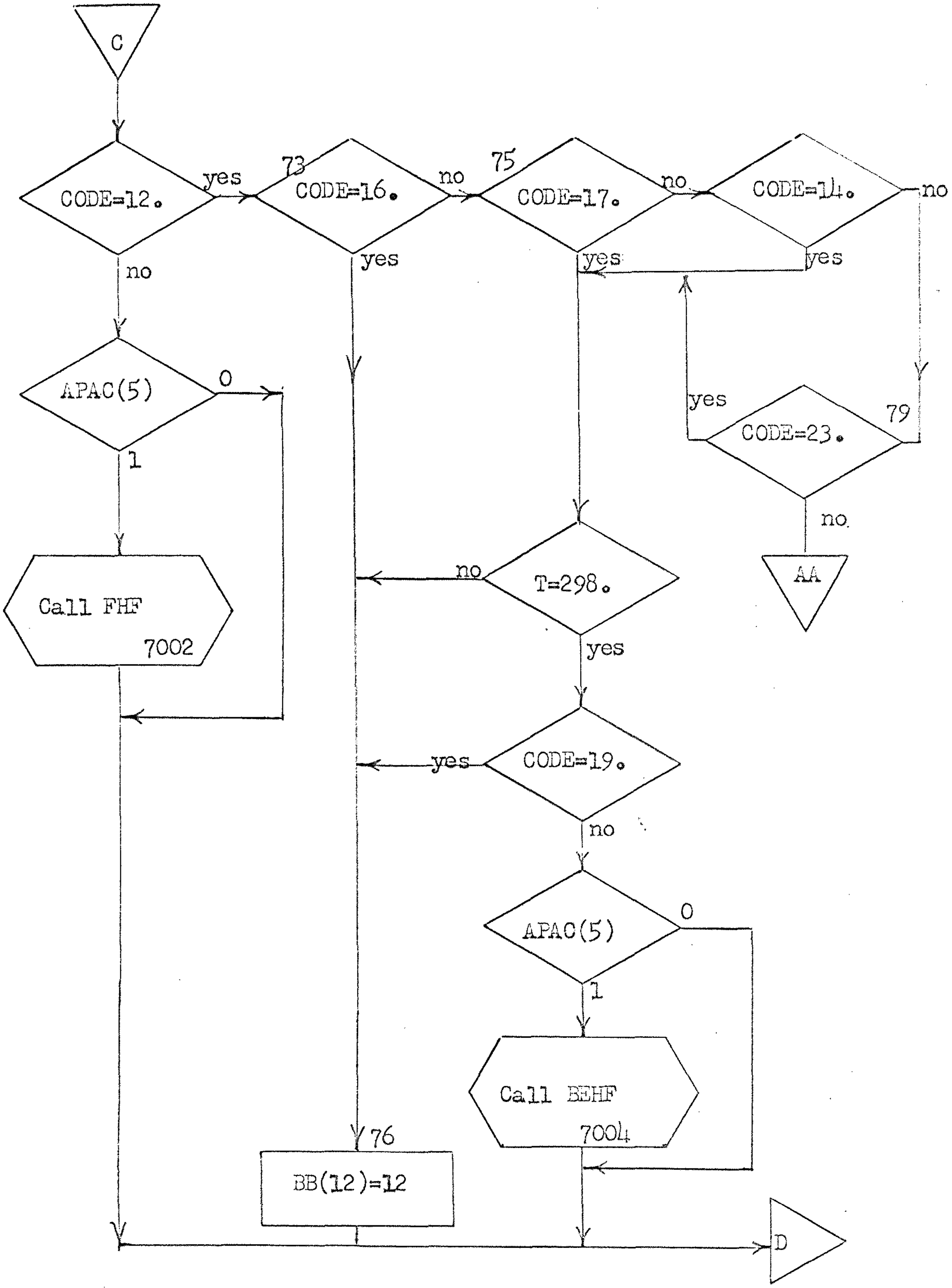
FLOW CHARTS FOR MAIN PROGRAM

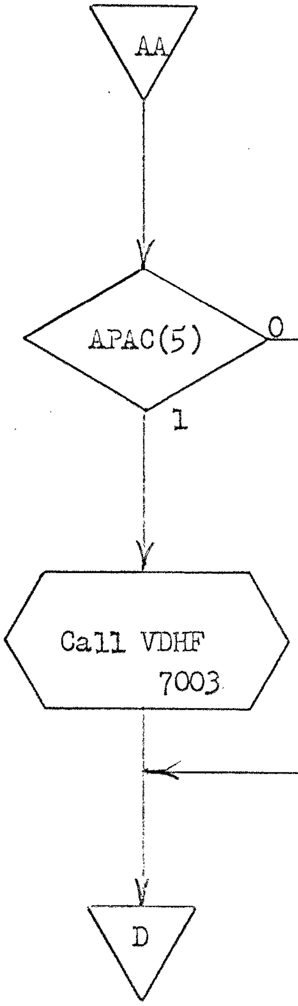


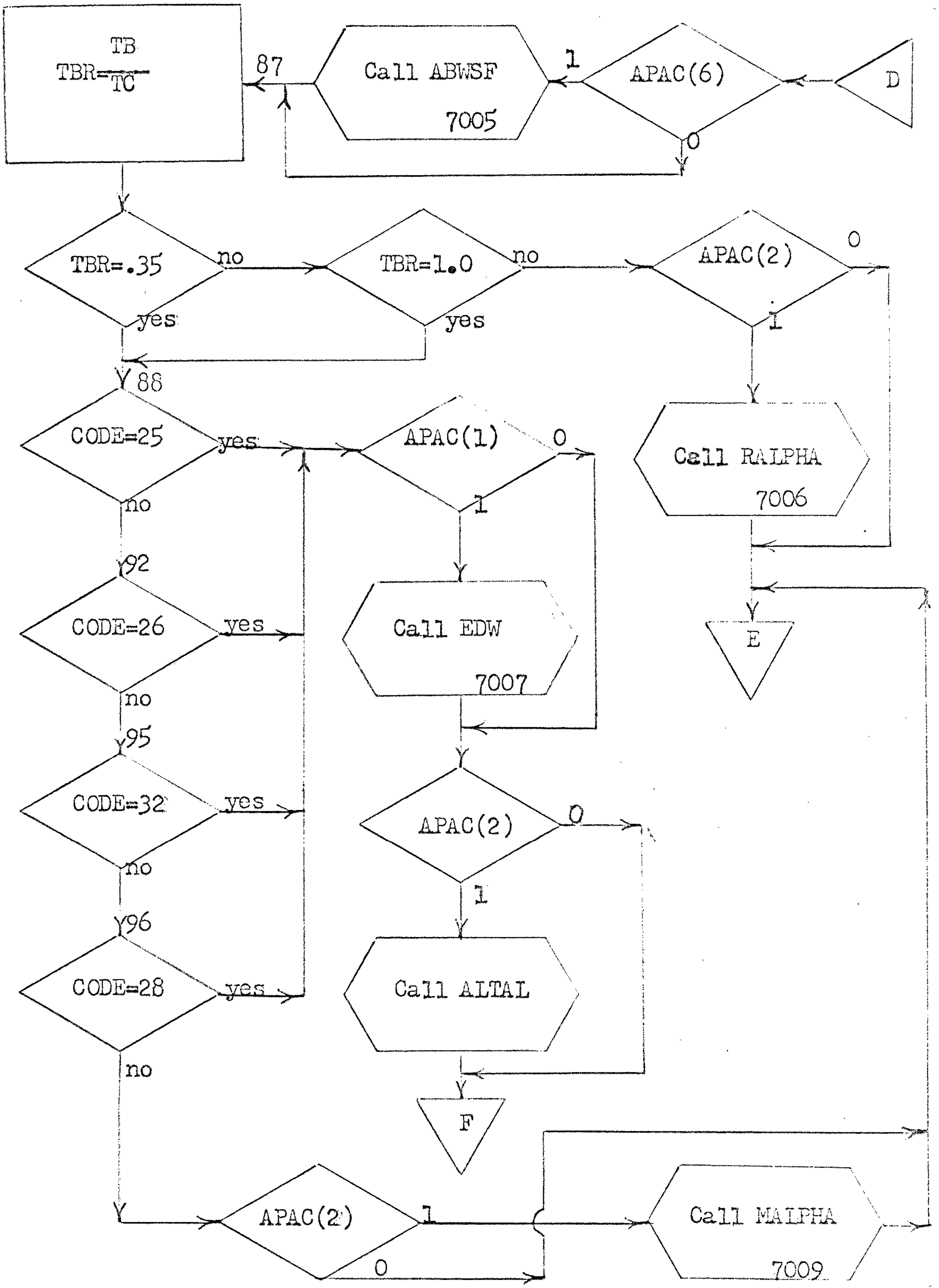

A
CALC
1
ZZZ
0
ALIQ
-
0
+
Call TBAC
APAC=read in
TB-T
-
APAC= read in
APAC(1-14)= 0.
0
+
APAC=read in
APAC(15-22)=0.
B

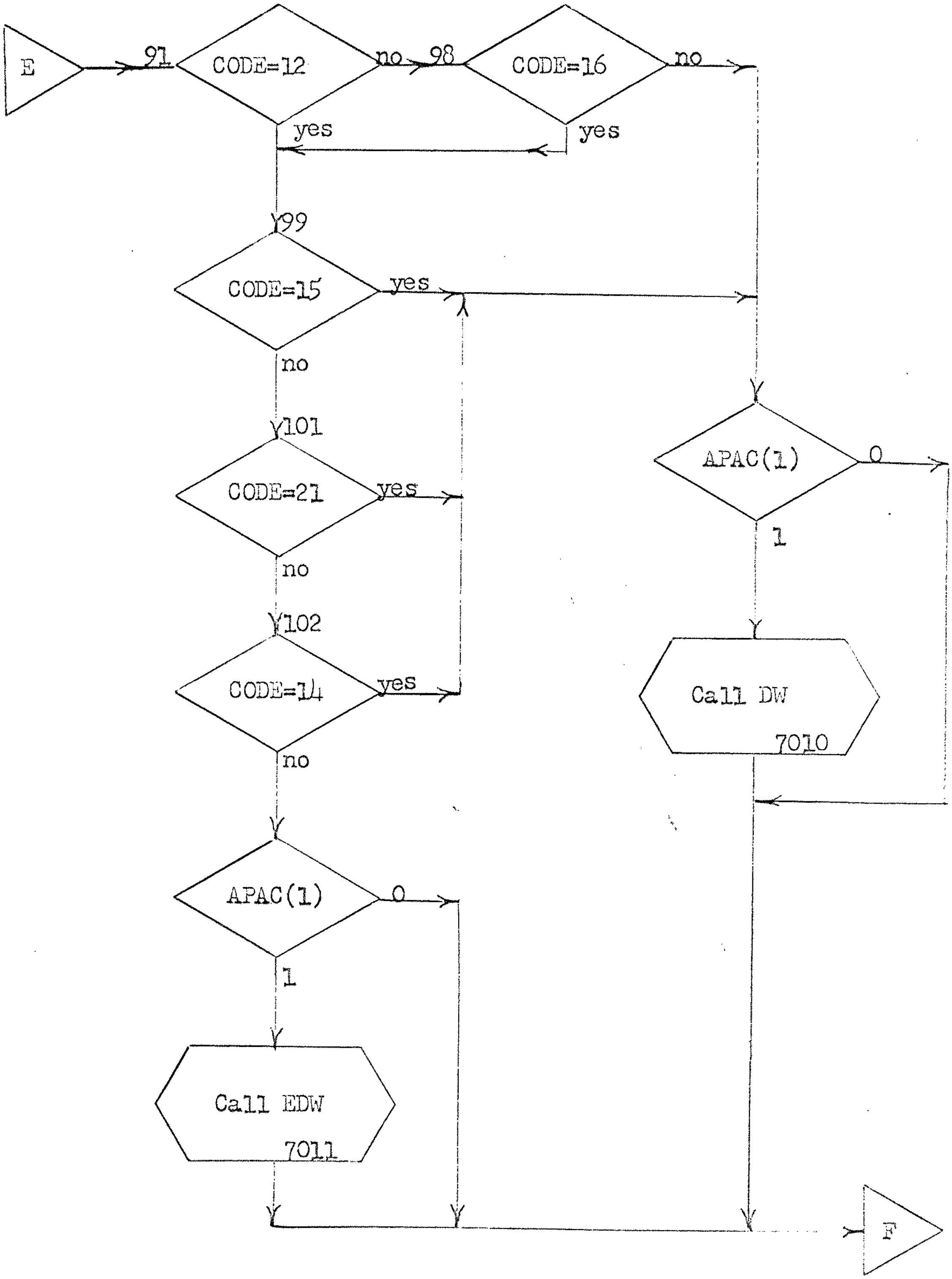

ZZZ
ALIQ
-
0
1
APAC(15-22)=1.
APAC(1-14)=0.
B
APAC(15-22)=0.
APAC(15-22)=0.
B
Call TBAC
TB-T
-
0
+

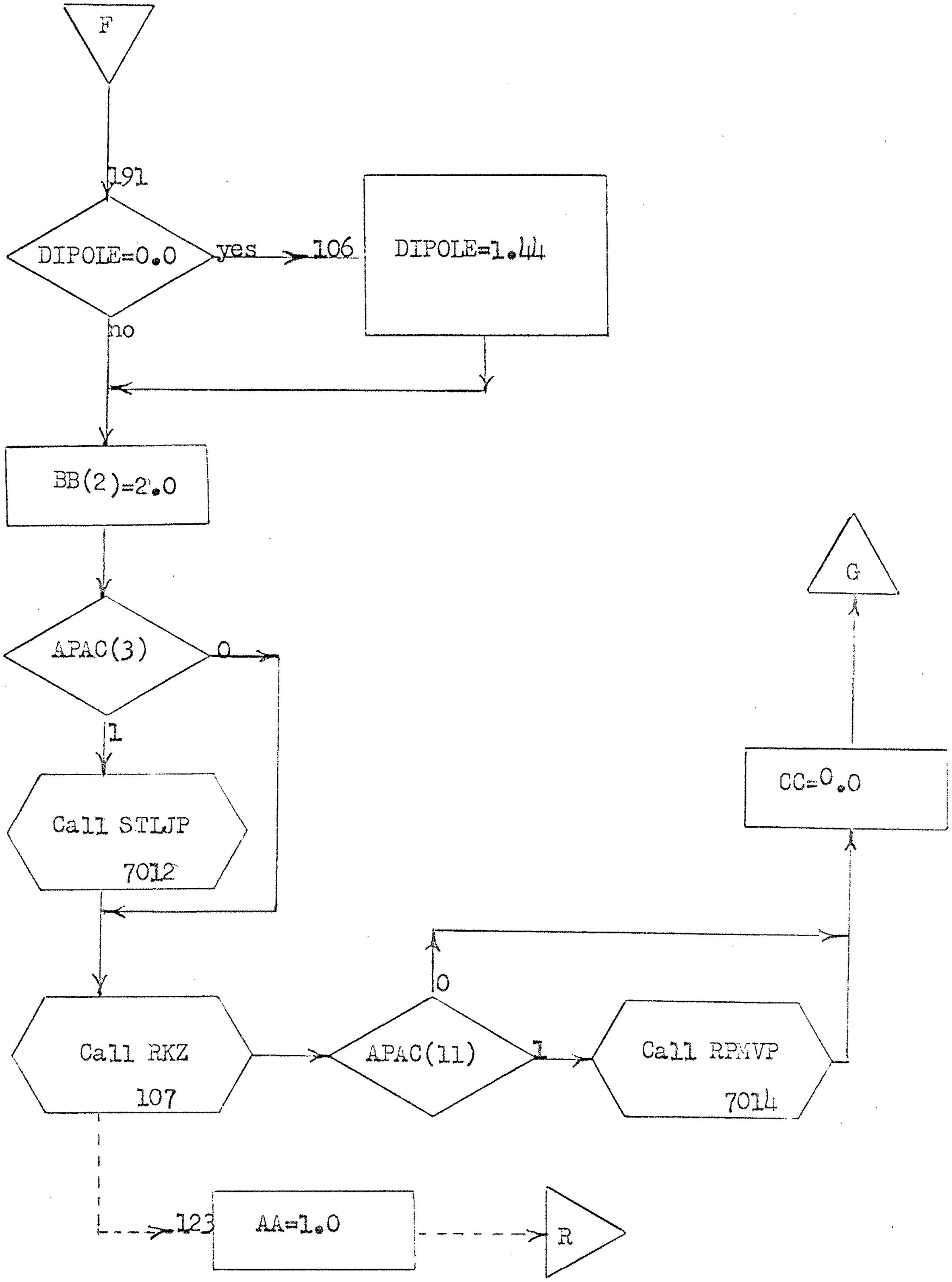

B
Convert AADAT And CADAT for individual subroutines
BB(J)=0.0
J=1,13
AA=0.0
Call PART 2
2222
CODE=7.
yes
no
66
CODE=21.
yes
no
68
CODE=24.
yes
no
67
CODE=15.
no
yes
71
BB(1)=1.0
APAC(4)
0
1
Call RDCPO
7000
APAC(4)
0
1
Call BRDCPO
7001
C

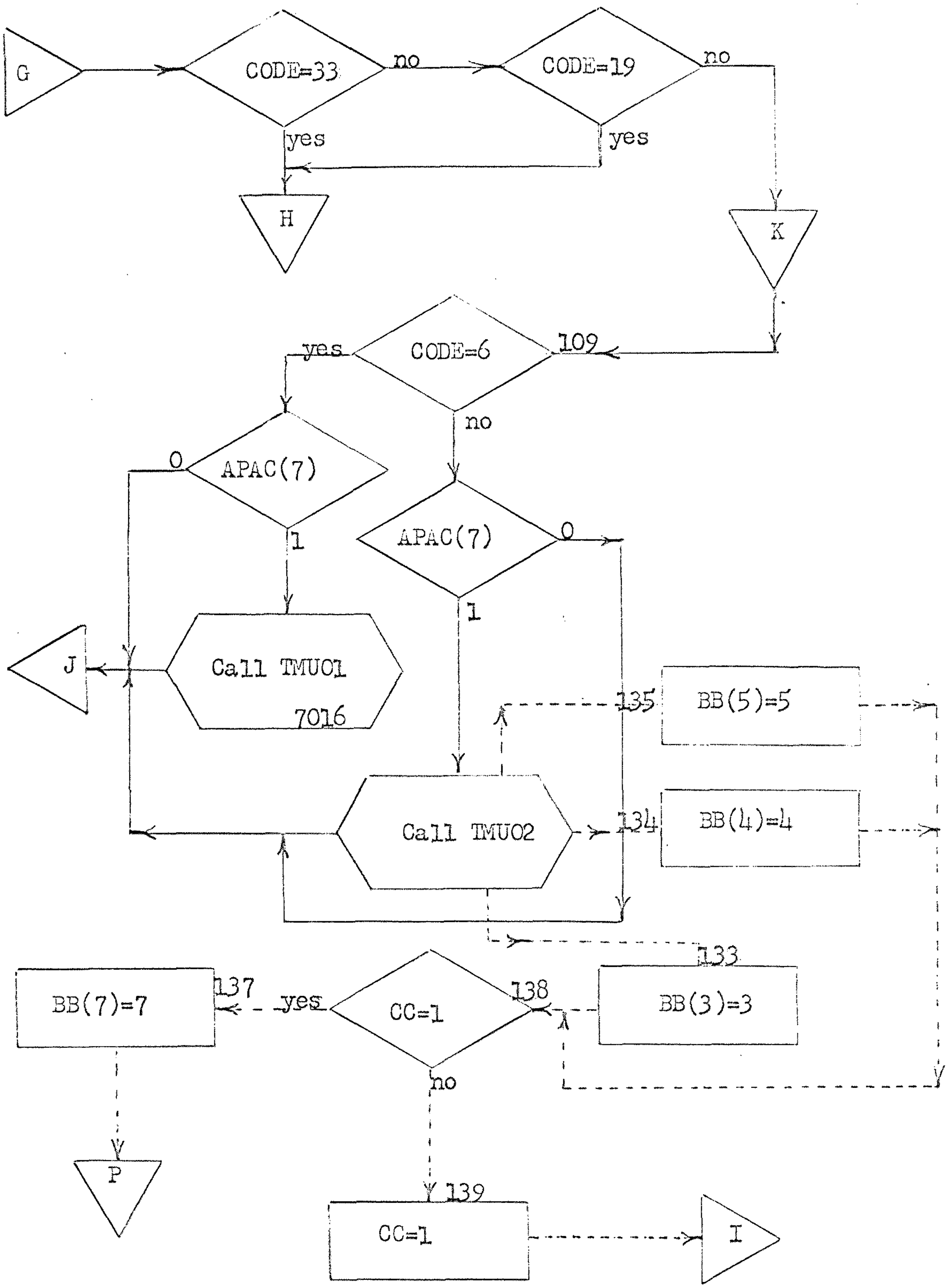

C
CODE=12.
yes
no
73
CODE=16.
no
yes
75
CODE=17.
no
yes
CODE=14.
no
yes
APAC(5)
0
1
Call FHF
7002
yes
79
CODE=23.
no
AA
no
T=298.
yes
yes
CODE=19.
no
APAC(5)
0
1
Call BEHF
7004
76
BB(12)=12
D

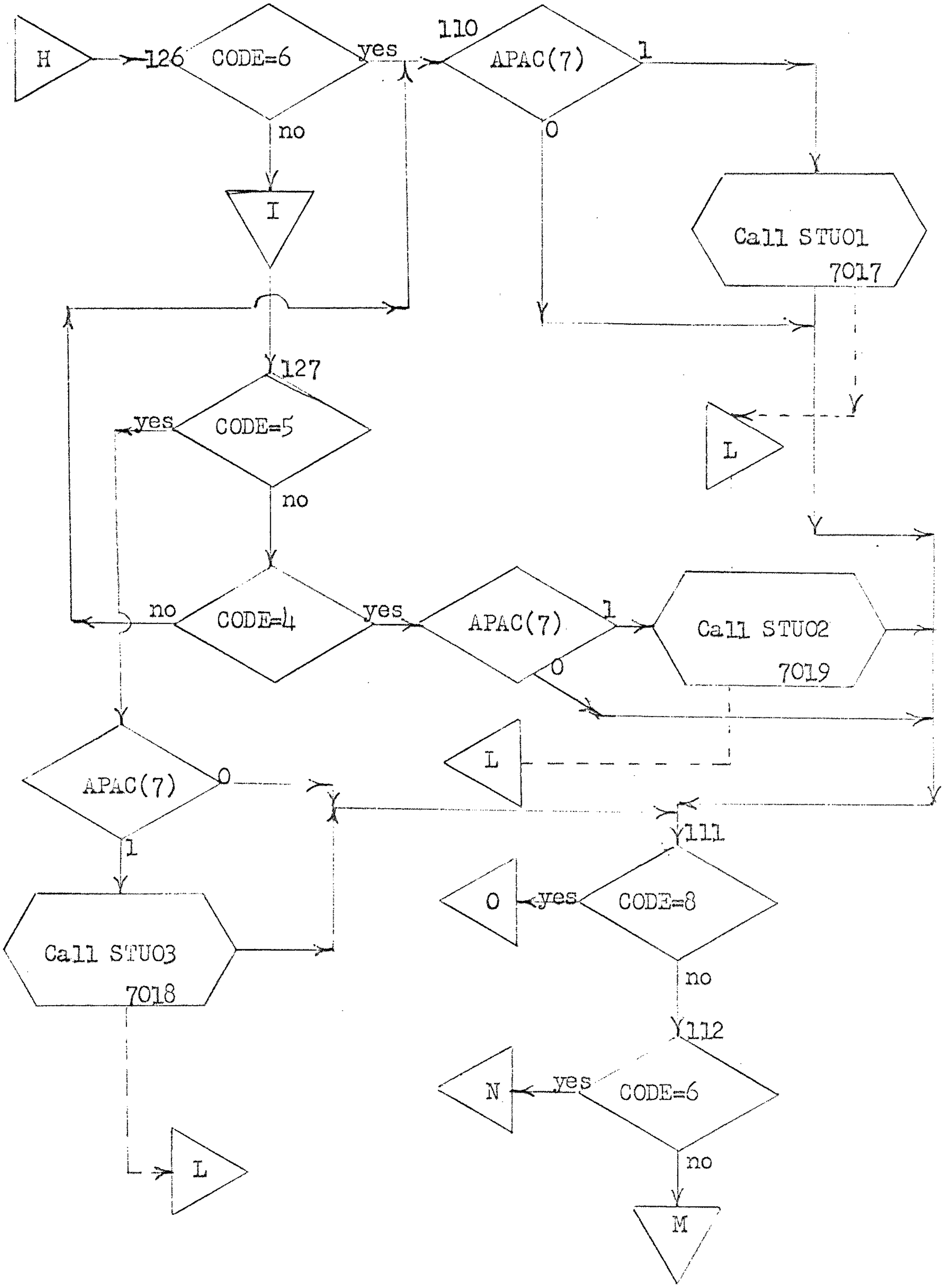

AA
APAC(5)
0
1
Call VDHF
7003
D

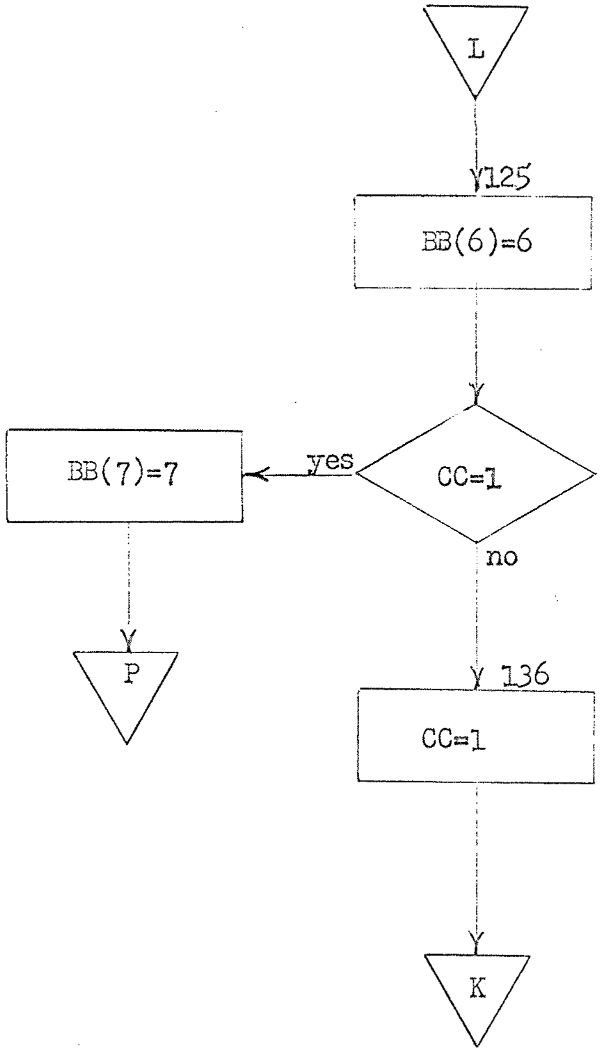

TBR= TB/TC
87
Call ABWSF
7005
1
APAC(6)
0
D
TBR=.35
no
yes
TBR=1.0
no
yes
APAC(2)
0
1
88
CODE=25
yes
no
APAC(1)
0
1
Call RALPHA
7006
92
CODE=26
yes
no
Call EDW
7007
E
95
CODE=32
yes
no
APAC(2)
0
1
96
CODE=28
yes
no
Call ALTAL
F
APAC(2)
1
0
Call MALPHA
7009

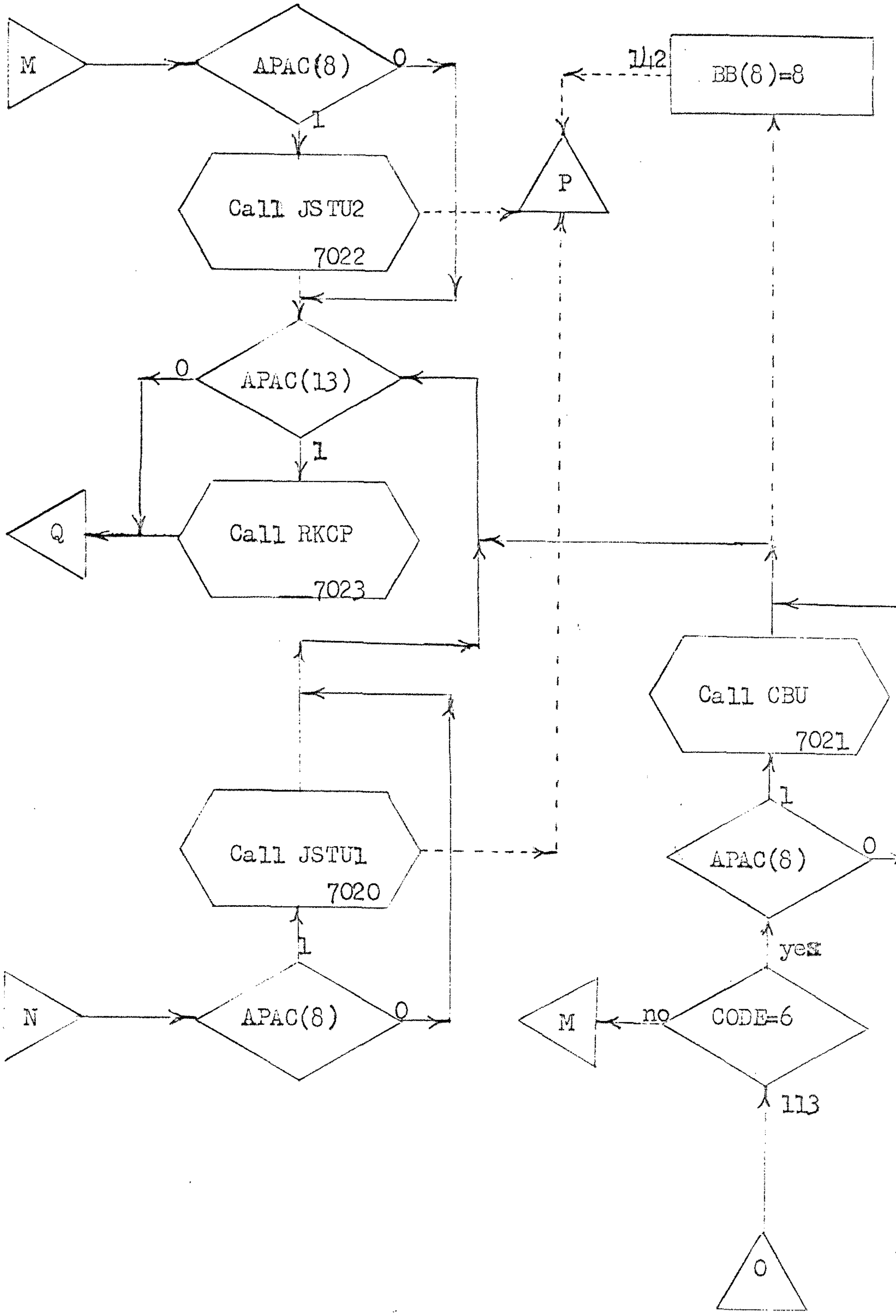

E
91
CODE=12
no
98
CODE=16
no
yes
yes
99
CODE=15
yes
no
101
CODE=21
yes
no
102
CODE=14
yes
no
APAC(1)
0
1
Call EDW
7011
APAC(1)
0
1
Call DW
7010
F

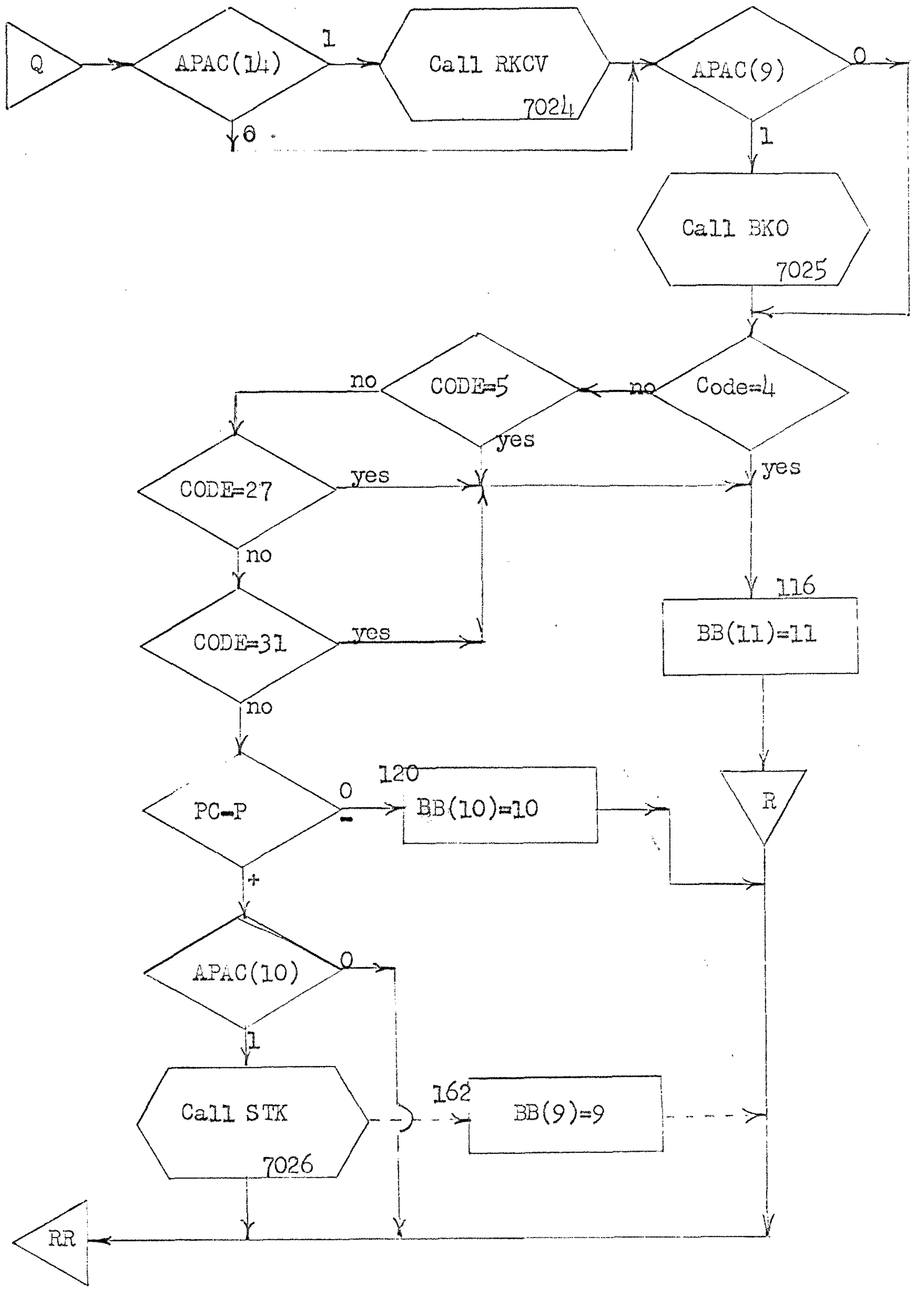

F
191
DIPOLE=0.0
yes
106
DIPOLE=1.44
no
BB(2)=2.0
APAC(3)
0
1
Call STLJP
7012
Call RKZ
107
APAC(11)
0
1
Call RPMVP
7014
CC=0.0
G
123
AA=1.0
R


G
CODE=33
no
yes
CODE=19
no
yes
H
K
CODE=6
109
yes
no
APAC(7)
0
1
APAC(7)
0
1
J
Call TMU01
7016
135
BB(5)=5
Call TMU02
134
BB(4)=4
133
BB(3)=3
BB(7)=7
137
yes
CC=1
138
no
P
139
CC=1
I


H
126
CODE=6
yes
no
I
110
APAC(7)
1
0
Call STU01
7017
L
127
CODE=5
yes
no
CODE=4
no
yes
APAC(7)
1
0
Call STU02
7019
L
APAC(7)
0
1
Call STU03
7018
L
111
CODE=8
yes
O
no
112
CODE=6
yes
N
no
M


L
125
BB(6)=6
CC=1
yes
no
BB(7)=7
P
136
CC=1
K


M
APAC(8)
0
1
142
BB(8)=8
Call JSTU2
7022
P
APAC(13)
0
1
Call RKCP
7023
Q
Call CBU
7021
Call JSTU1
7020
1
APAC(8)
0
N
APAC(8)
0
yes
M
no
CODE=6
113
O


Q
APAC(14)
1
0
Call RKCV
7024
APAC(9)
0
1
Call BKO
7025
Code=4
no
yes
CODE=5
no
yes
CODE=27
yes
no
CODE=31
yes
no
116
BB(11)=11
R
PC-P
0
-
120
BB(10)=10
+
APAC(10)
0
1
Call STK
7026
162
BB(9)=9
RR

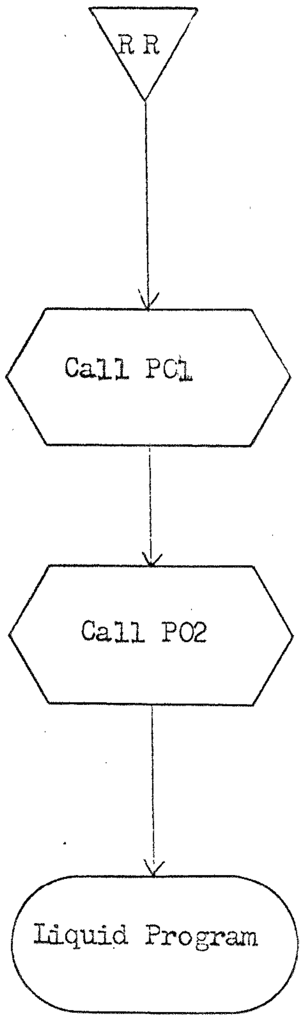

R R
Call PC1
Call PO2
Liquid Program

FIGURE 1 (Cont.)

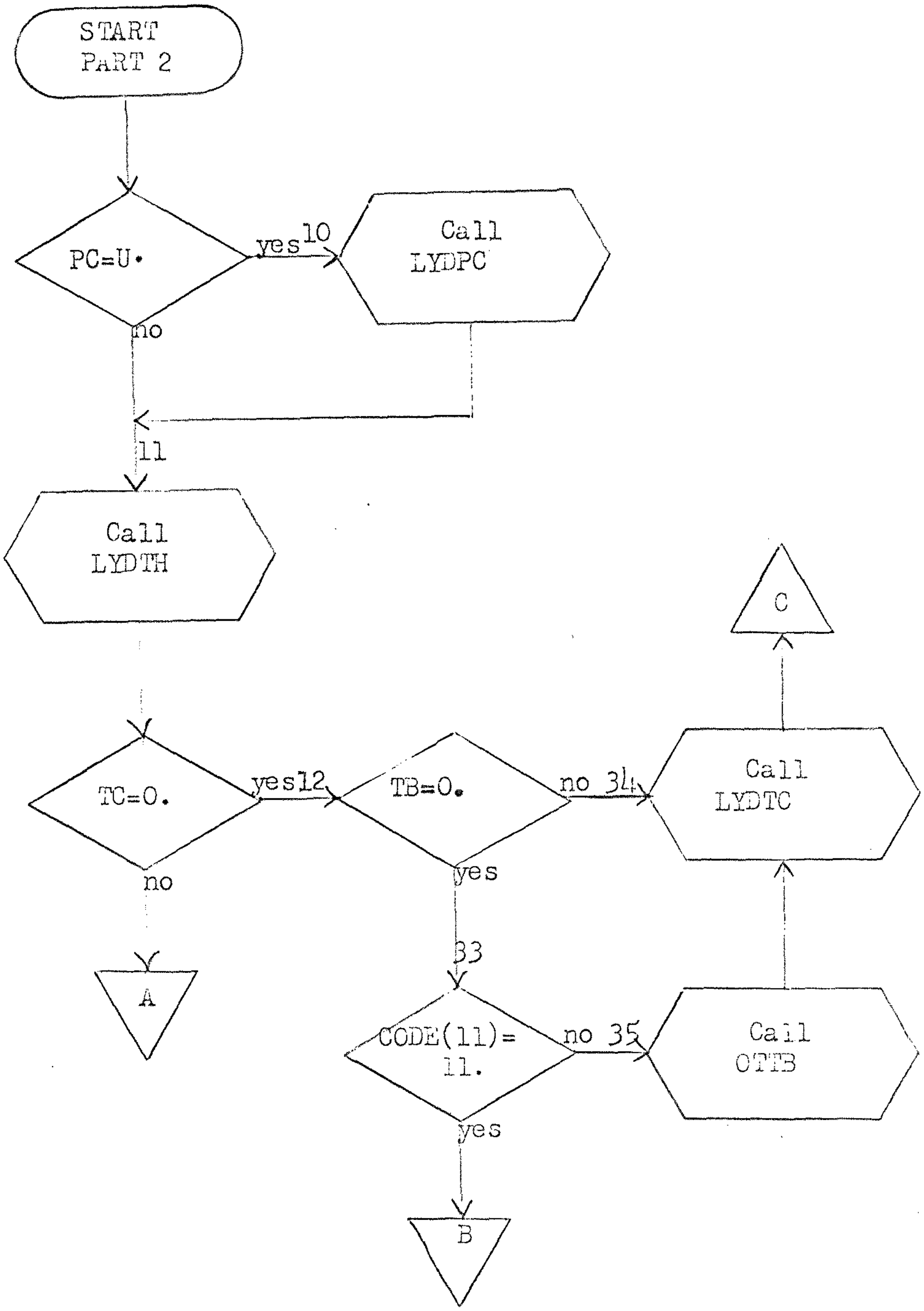


FIGURE 1 (Cont.)

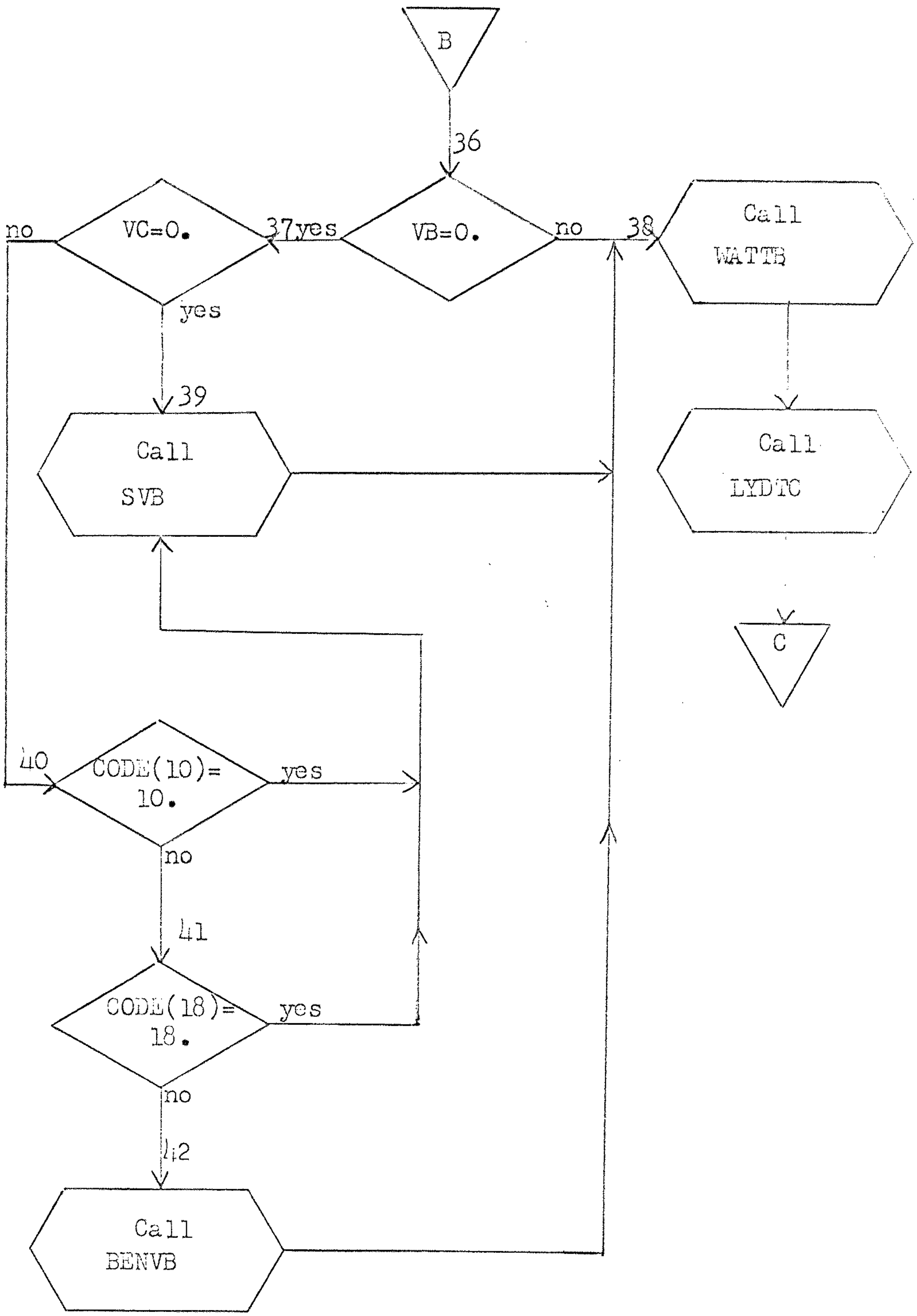


FIGURE 1 (Cont.)

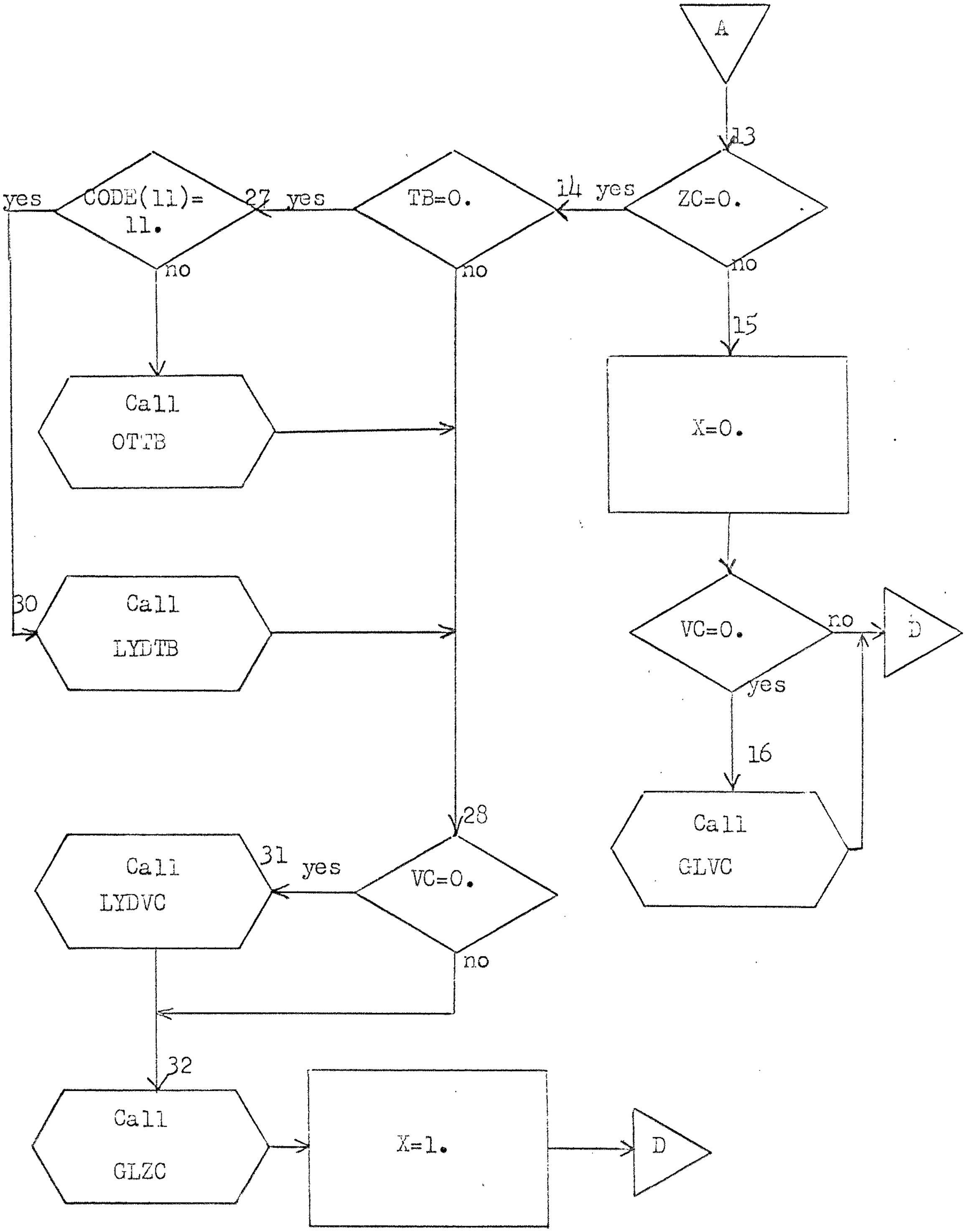


FIGURE 1 (Cont.)

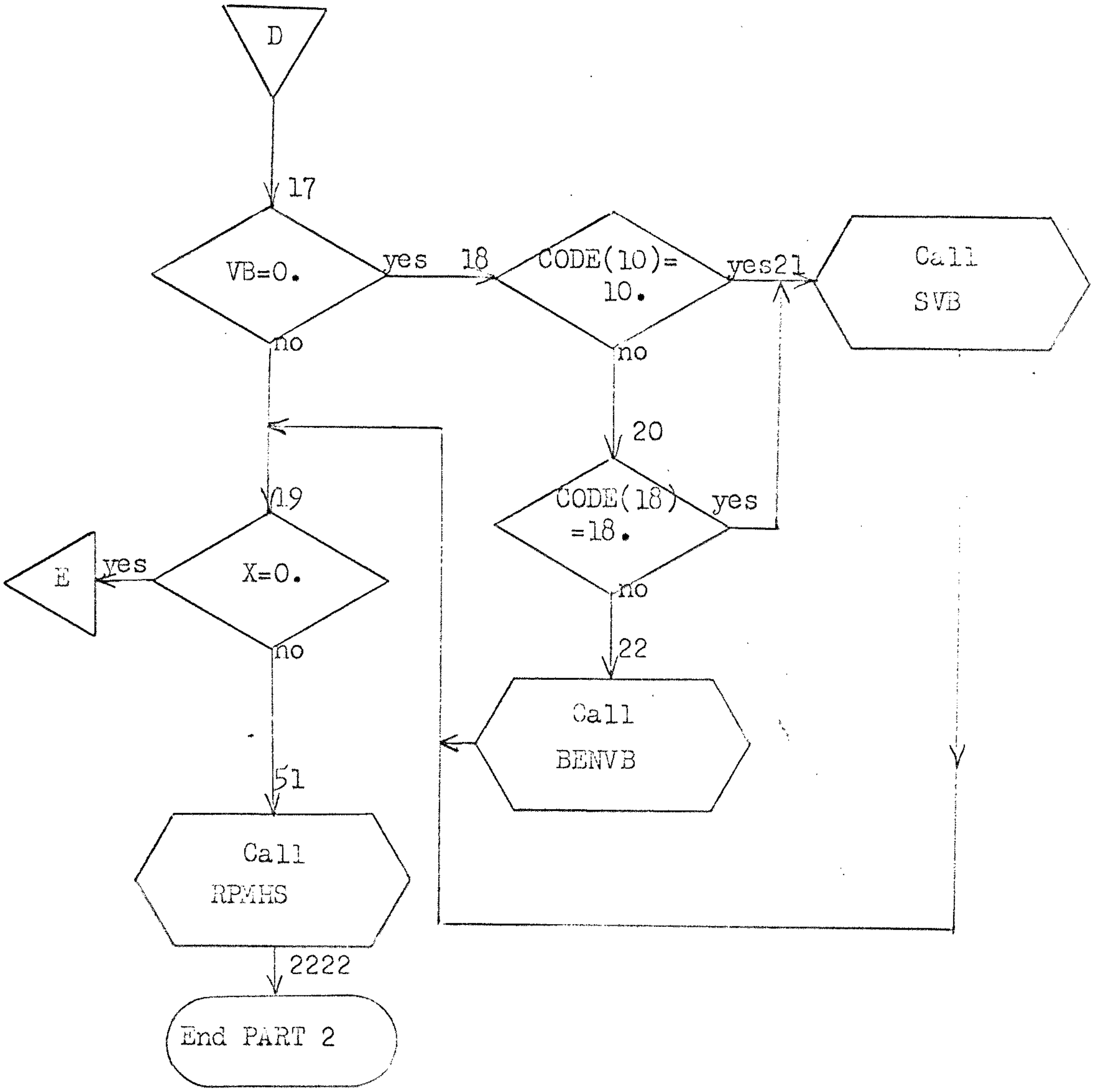


FIGURE 1 (Cont.)

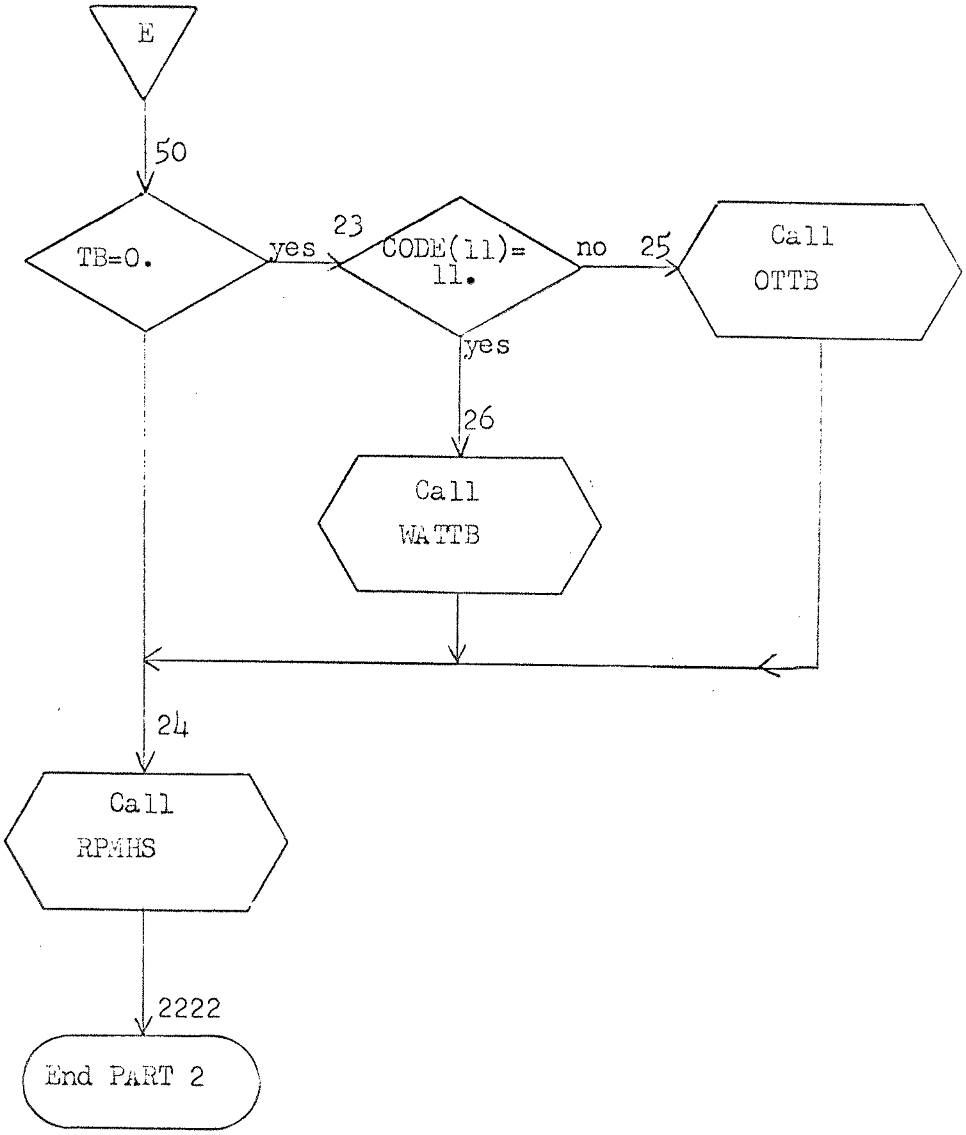


FIGURE 1 (Cont.)

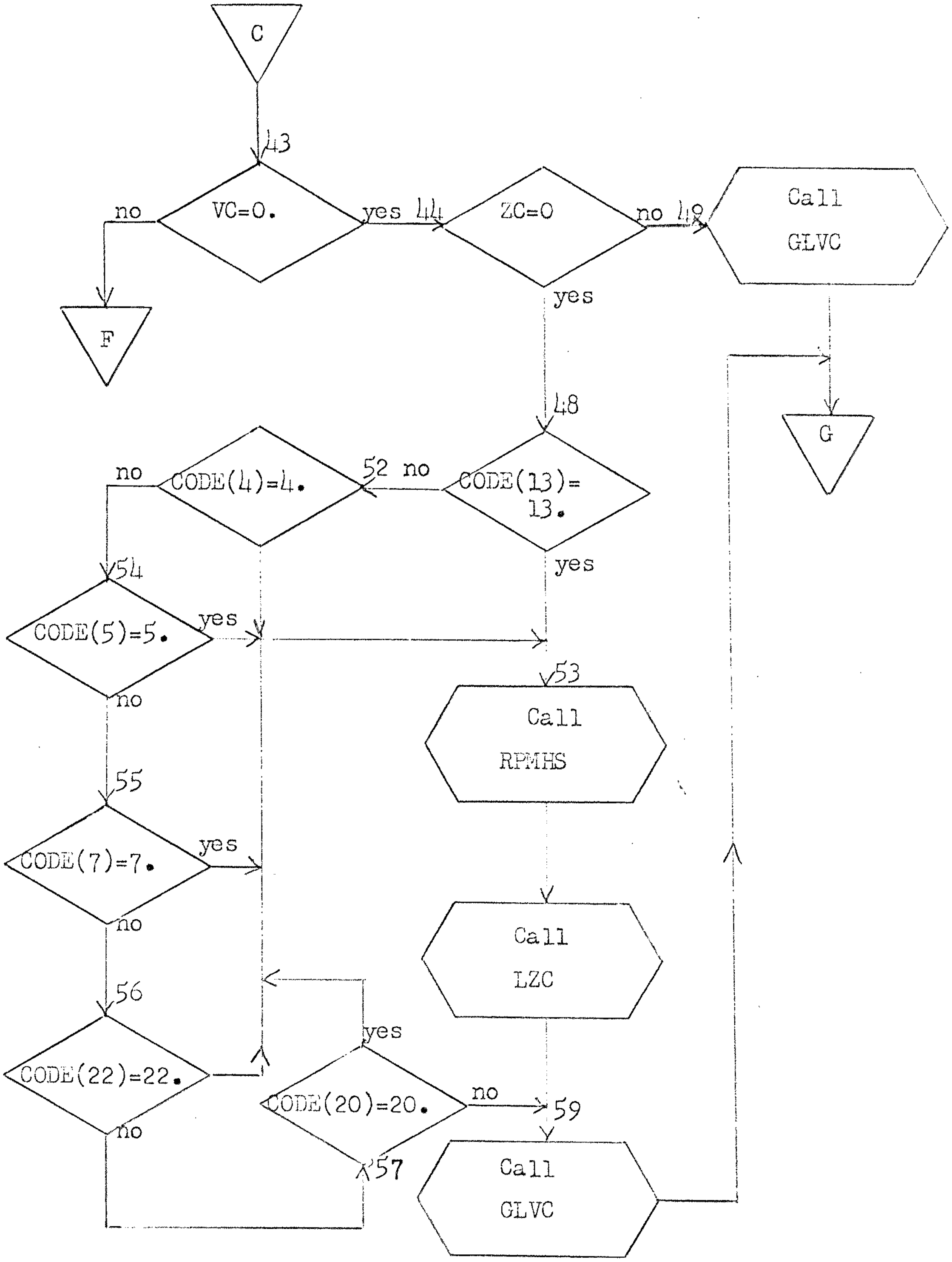
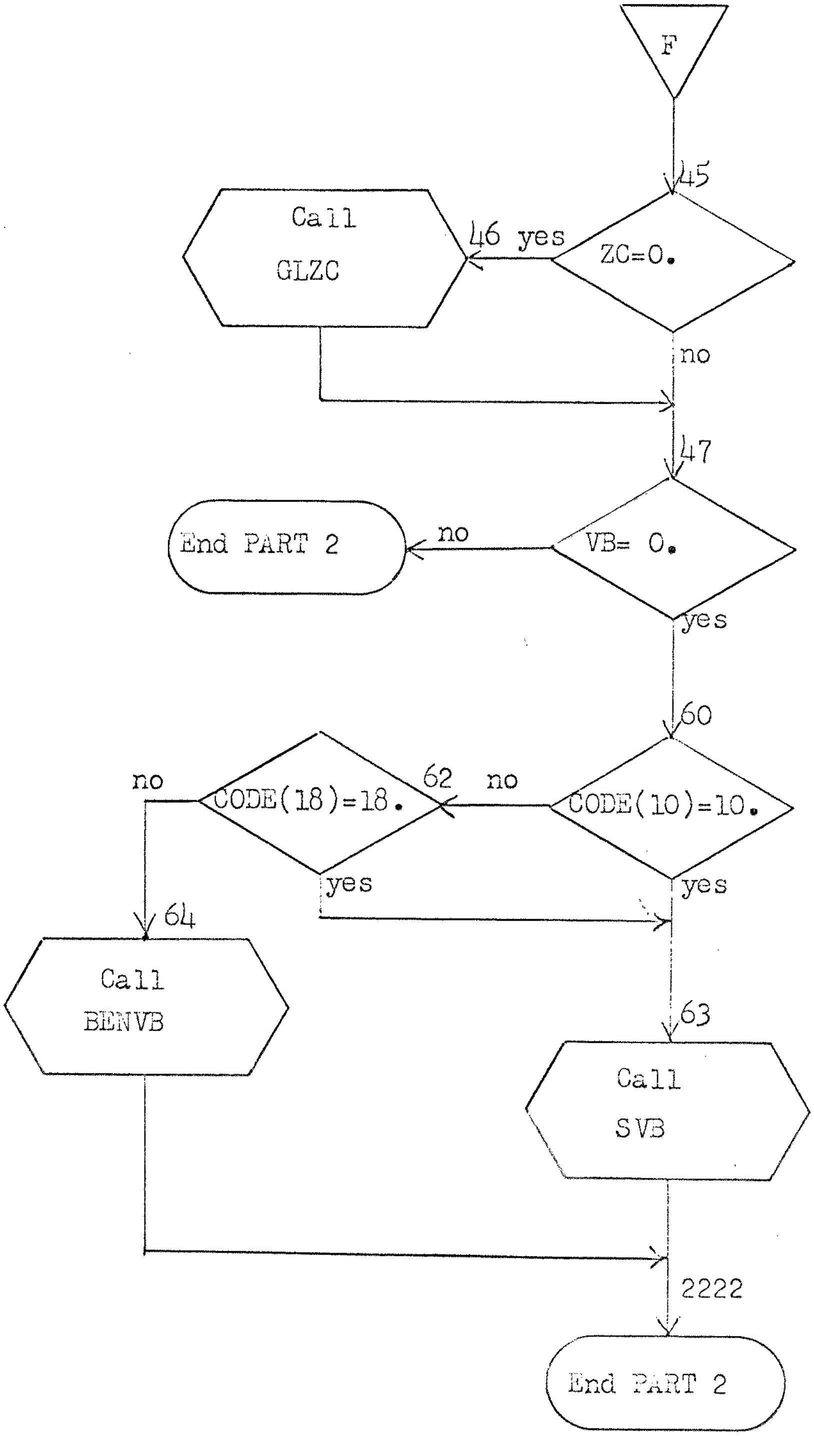
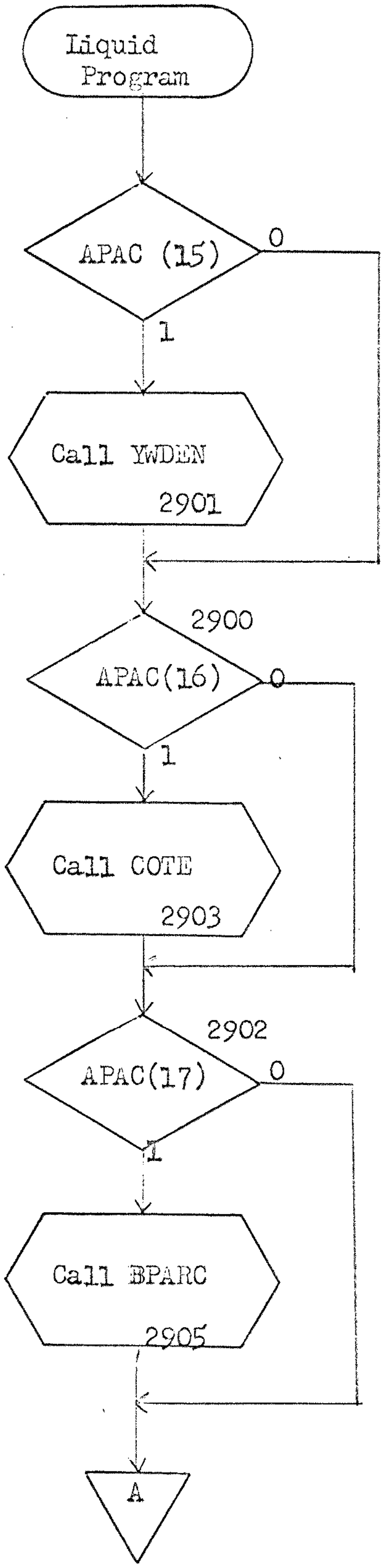
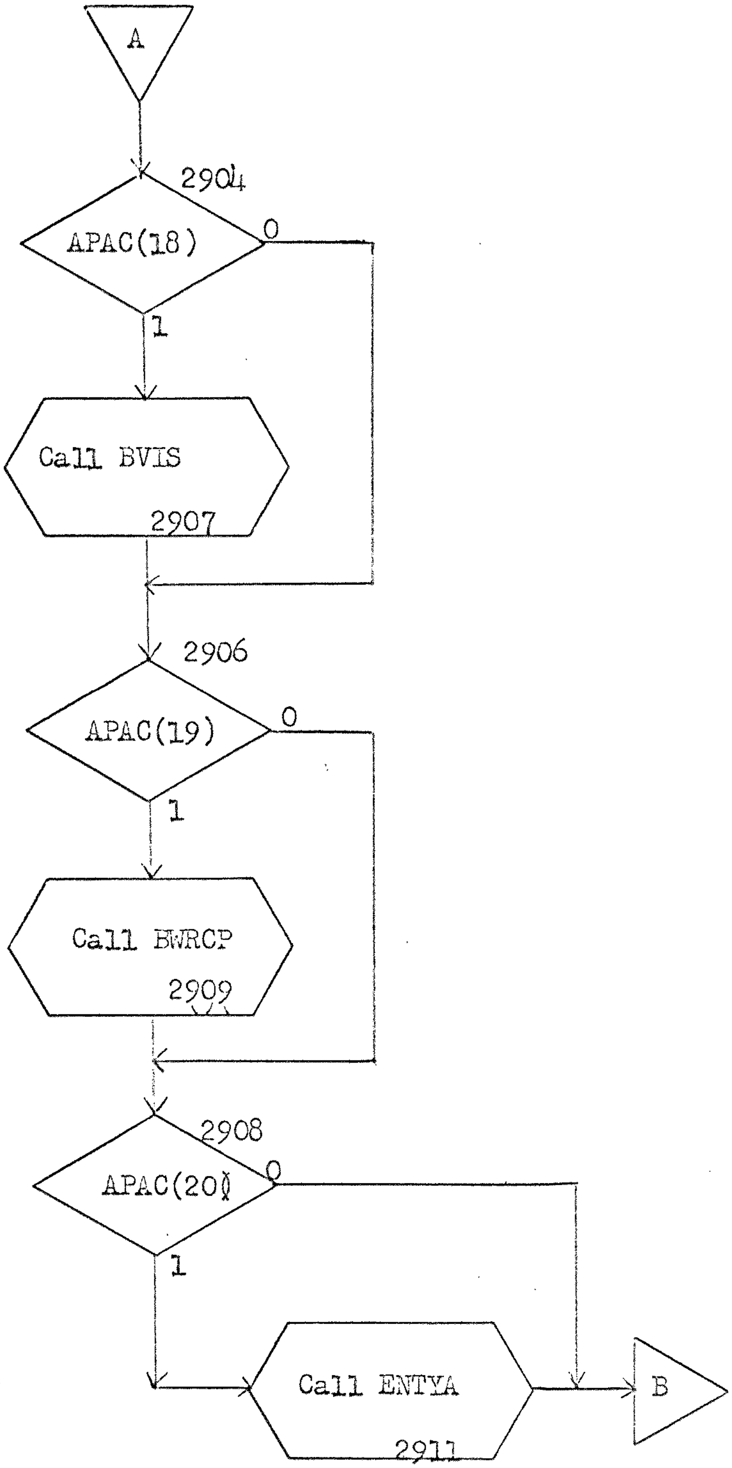


FIGURE 1 (Cont.)




Liquid Program
APAC (15)
0
1
Call YWDEN
2901
2900
APAC(16)
0
1
Call COTE
2903
2902
APAC(17)
0
1
Call BPARC
2905
A


A
2904
APAC(18)
0
1
Call BVIS
2907
2906
APAC(19)
0
1
Call BWRCP
2909
2908
APAC(20)
0
1
Call ENTYA
2911
B

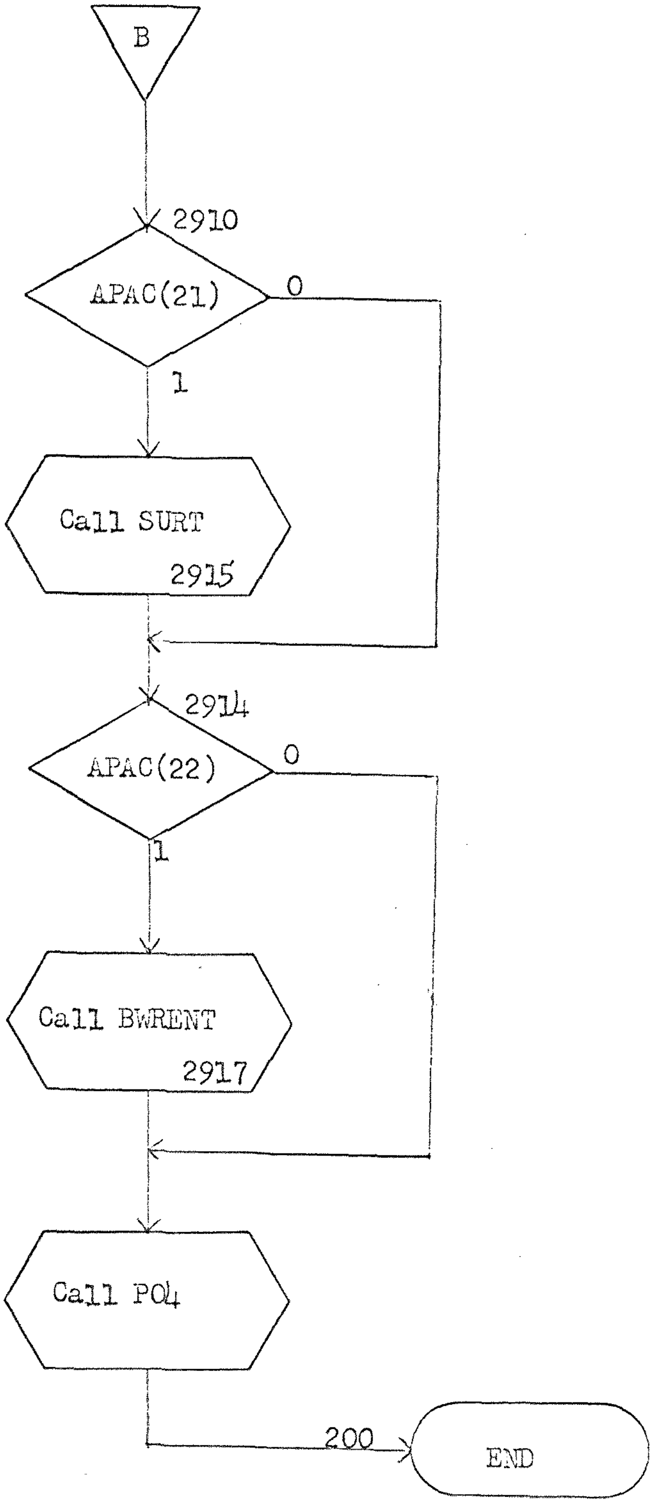

B
2910
APAC(21)
0
1
Call SURT
2915
2914
APAC(22)
0
1
Call BWRENT
2917
Call PO4
200
END

FIGURE 2

FLOW CHART FOR PRINT OUT PART ONE

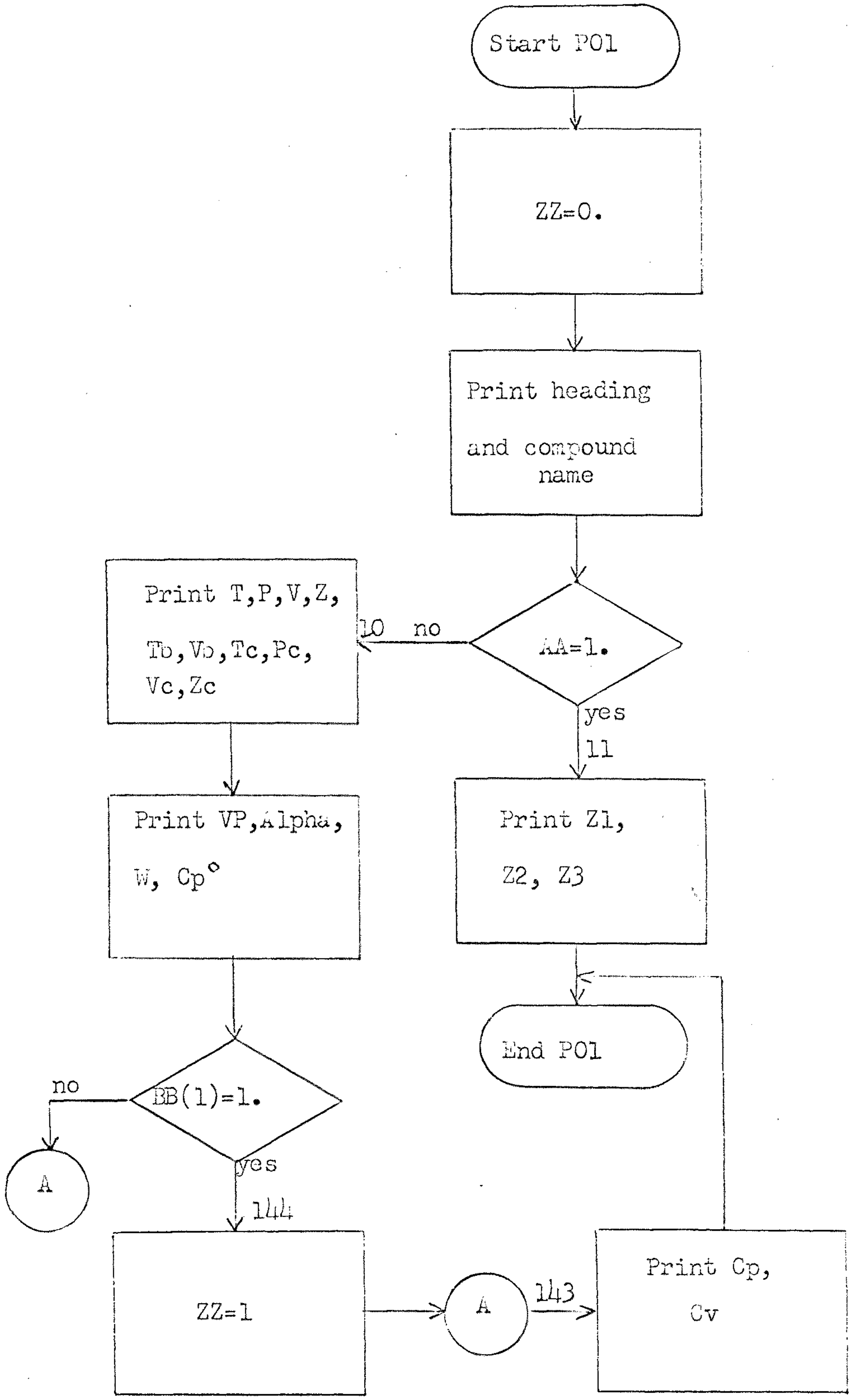


FIGURE 3

FLOW CHART FOR PRINT OUT PART TWO

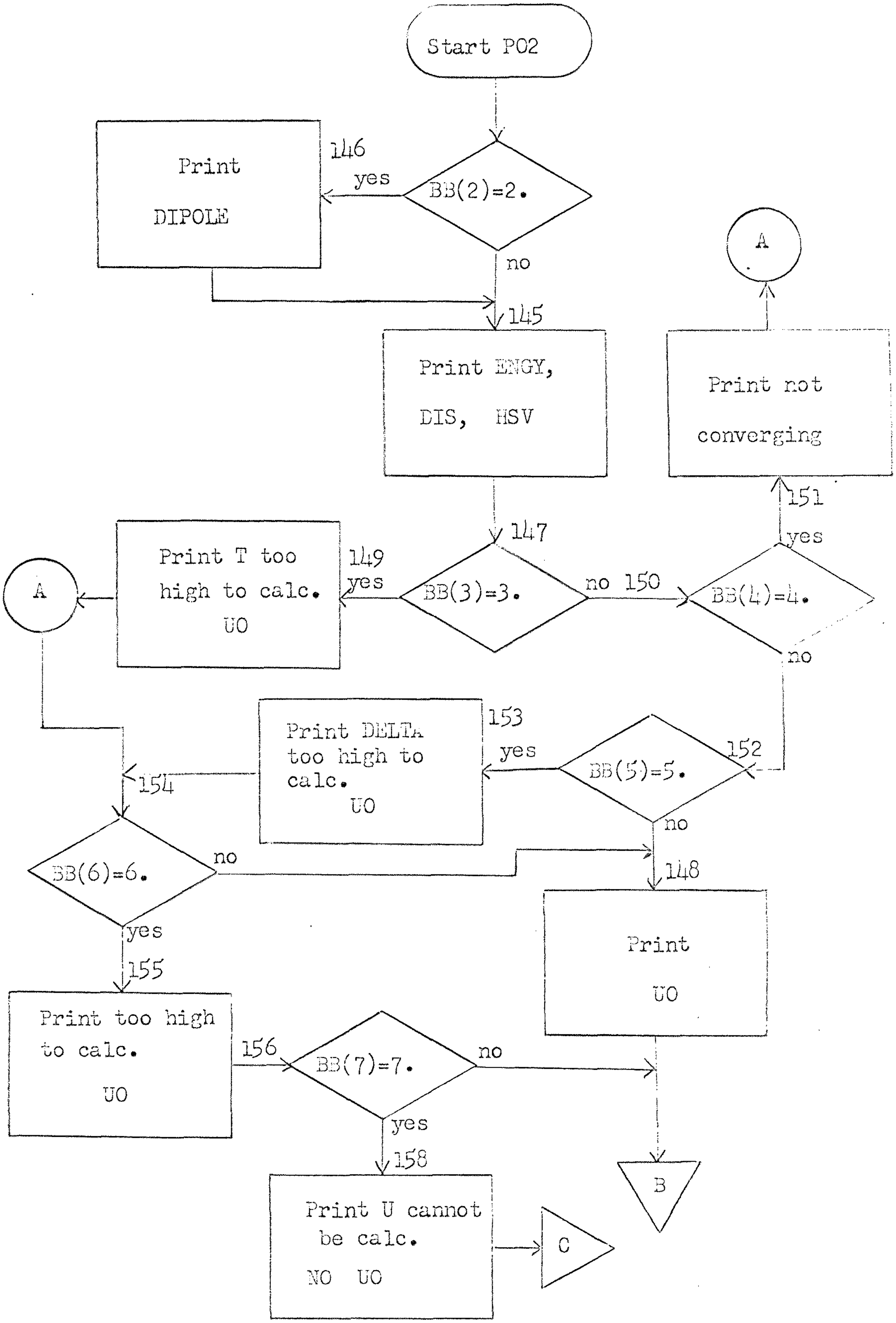


FIGURE 3 (Cont.)

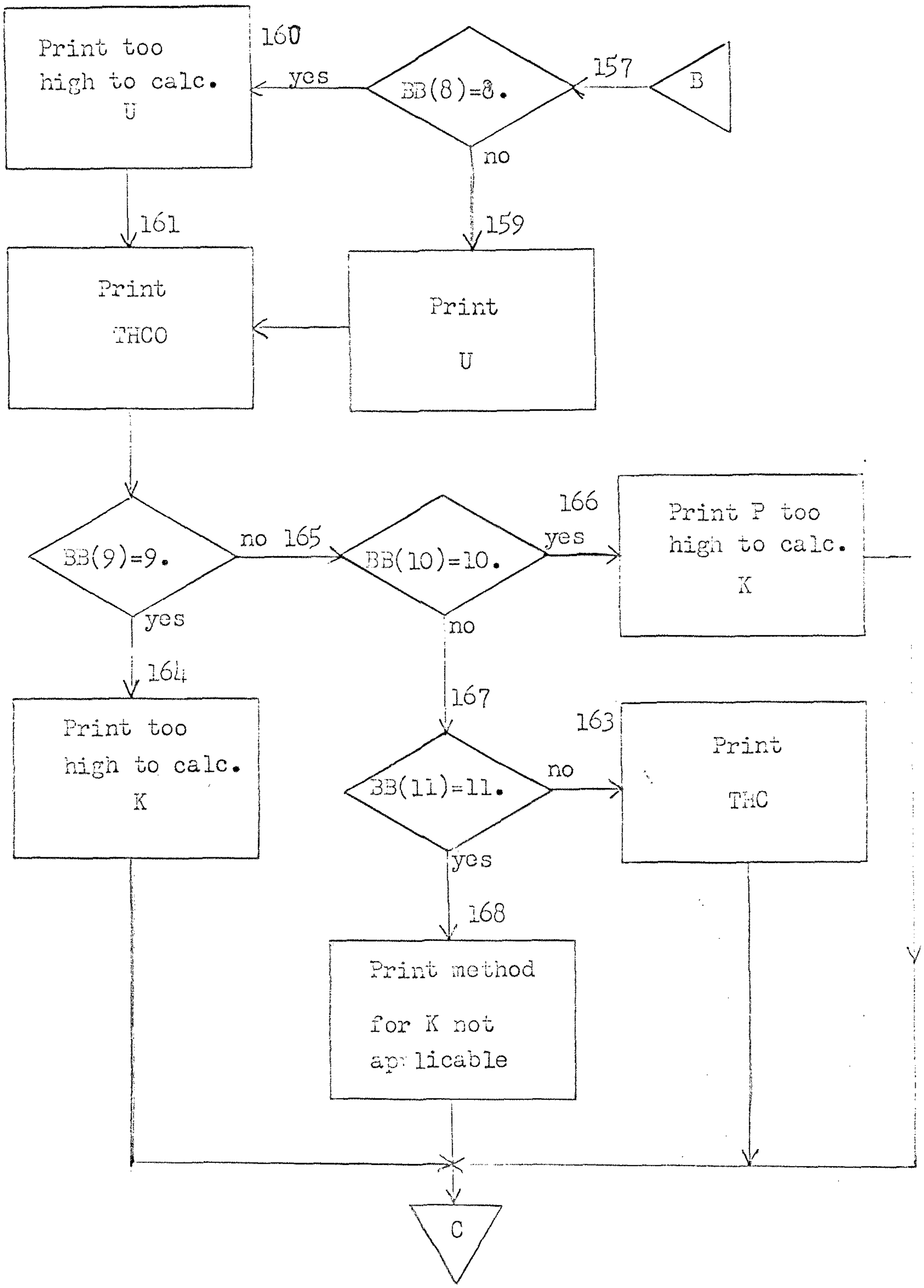
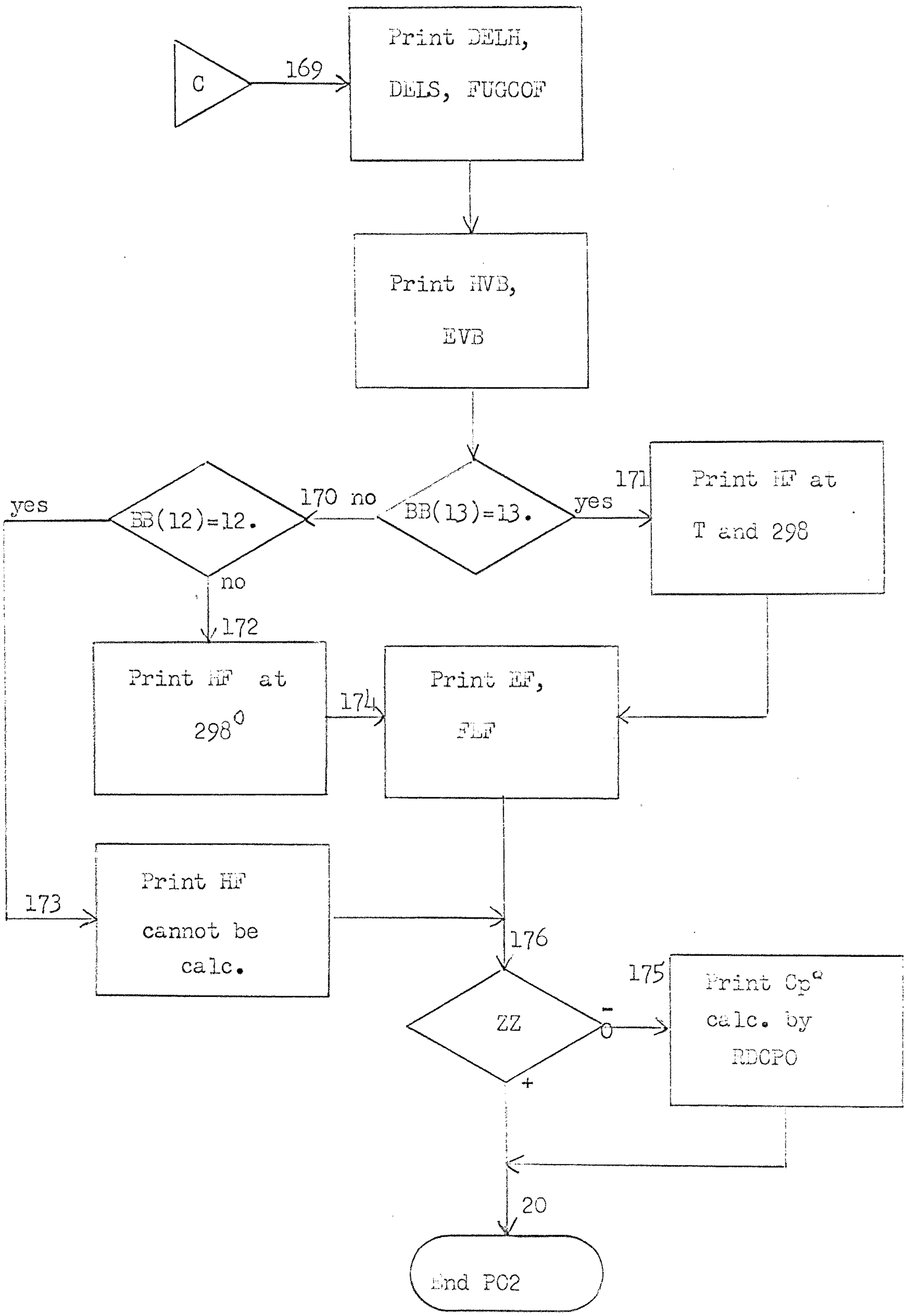
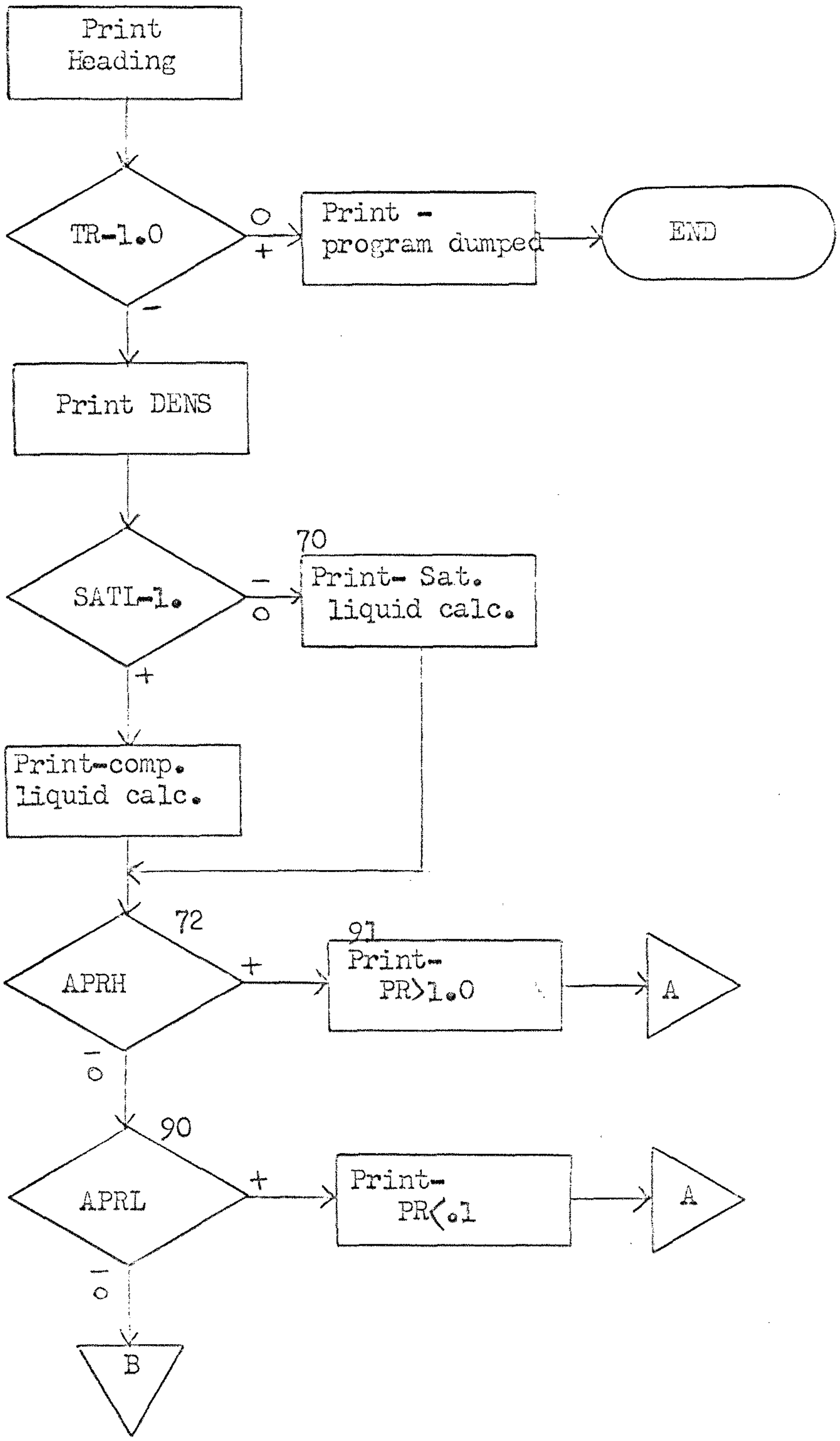
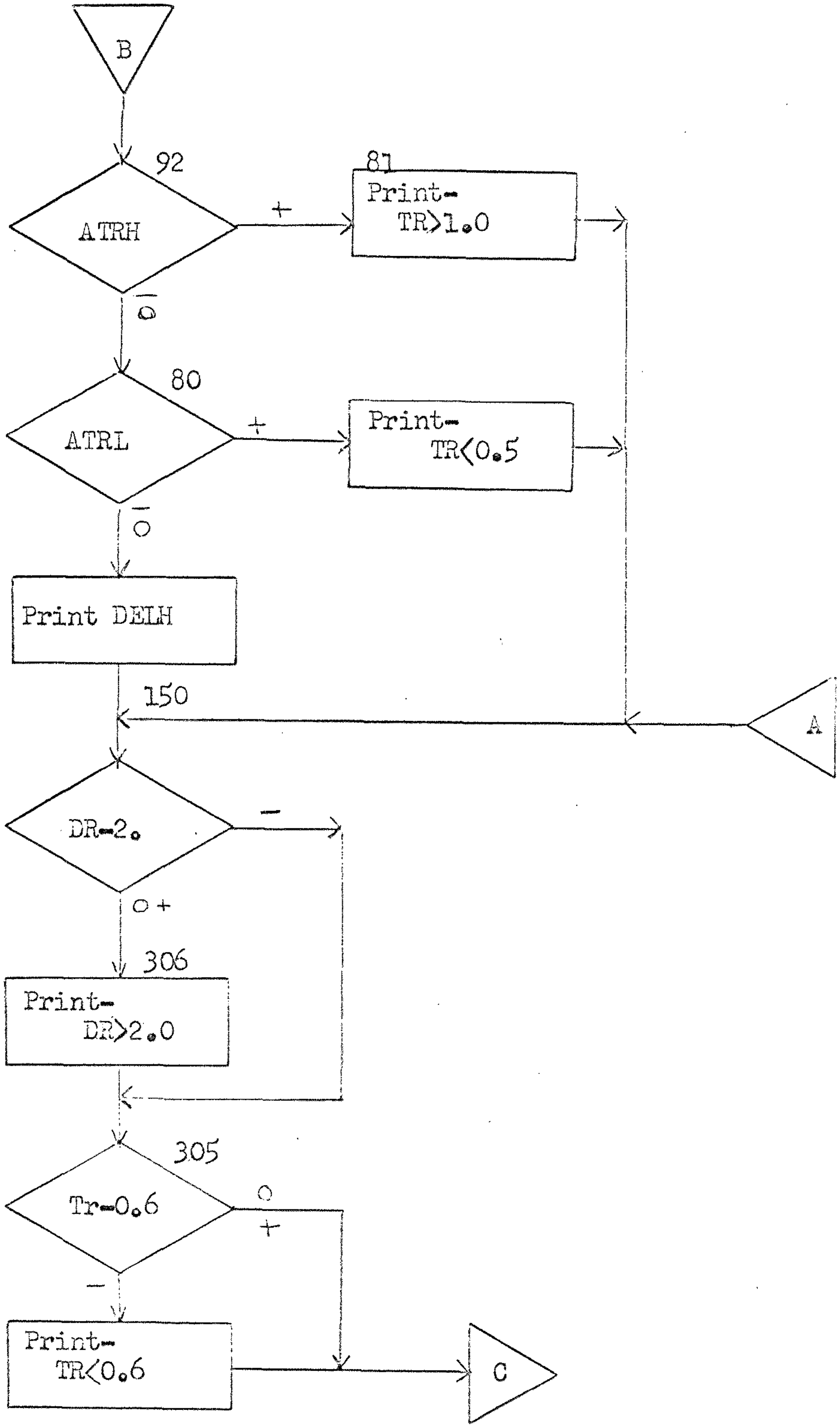


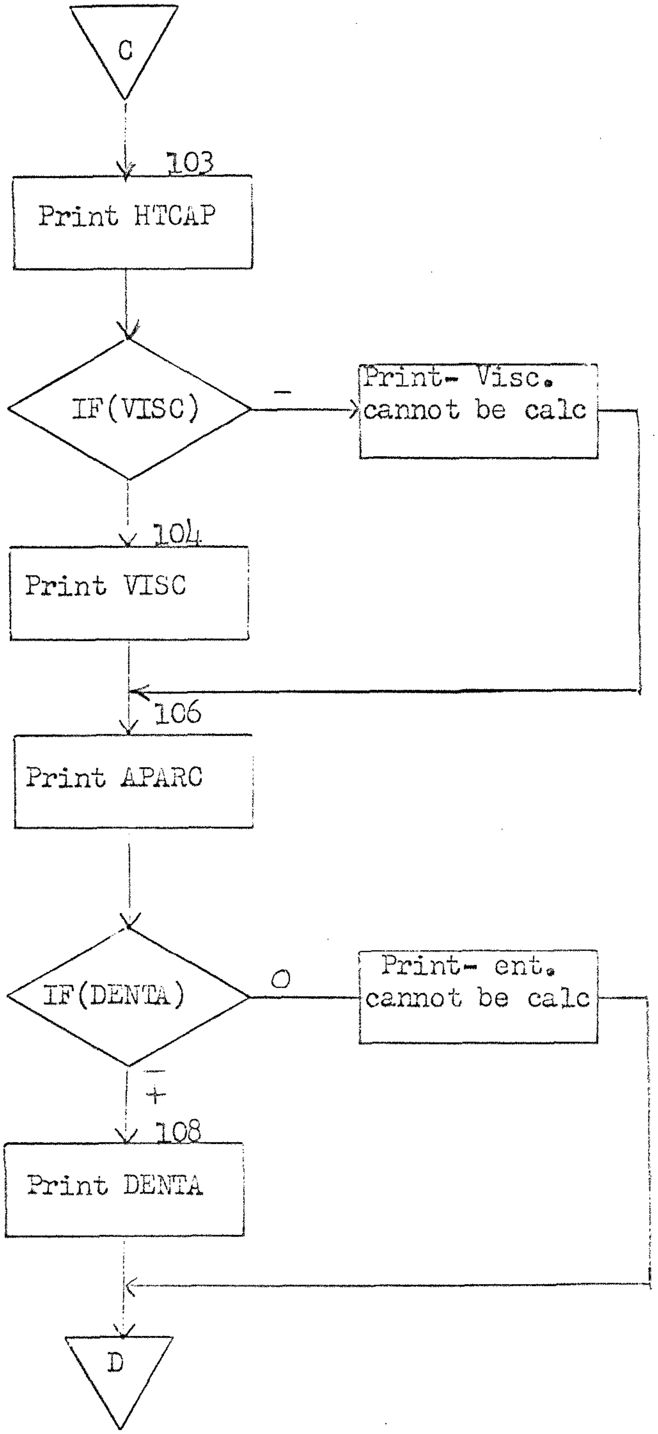
FIGURE 3 (Cont.)

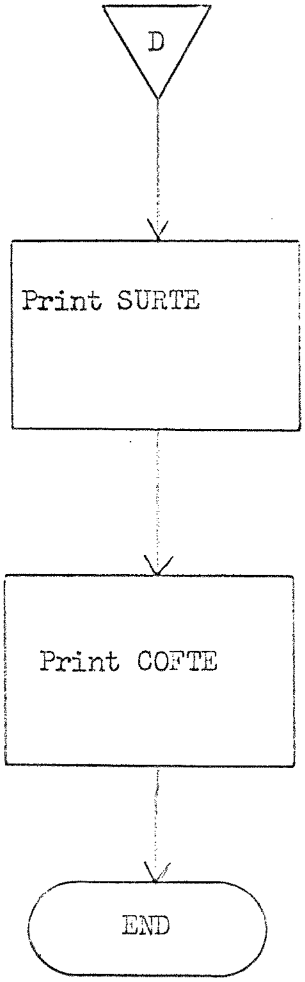


FLOW CHART FOR PRINT OUT PART 4




B
92
ATRH
+
81
Print-
TR>1.0
0
80
ATRL
+
Print-
TR<0.5
0
Print DELH
150
A
DR-2.
−
0 +
306
Print-
DR>2.0
305
Tr-0.6
0
+
−
Print-
TR<0.6
C


C
103
Print HTCAP
IF(VISC)
−
Print- Visc.
cannot be calc
104
Print VISC
106
Print APARC
IF(DENTA)
0
Print- ent.
cannot be calc
−
+
108
Print DENTA
D


D
Print SURTE
Print COFTE
END

USE OF PROGRAM

There are two input data sections in the estimation program (see program structure for description). The first consists of internal arrays for the consolidated input AADAT, tables of group contributions (AMCGC thru Y), setting all physical properties at a value of 0.0 (TC thru COFTL) and the logic for calculating single physical properties (APA(N,1), APA(N,2)). This body of common data is read in each time the program is run except when:

> physical properties are estimated at various combinations of temperature and pressure (PN is greater than 1); and during a single run, various compounds will be estimated as signified by reading the appropriate value for N.

The second part of the data input is peculiar to each compound being estimated. An example of a data set is illustrated and explained below for acetic acid.

Input

N - Since only one compound is being considered, a value of 1 is is input and the program will only input one set of the following data.

NAME - The compound name is input:

ACETIC ACID

WT - The molecular weight of acetic acid is input:

60.05

CODE (Table III, page 68) - Input the numbers of the pertinent descriptions:

```
0.0     2.0     0.0     4.0     0.0     0.0     0.0     0.0
9.0     0.0    11.0     0.0     0.0     0.0     0.0     0.0
0.0     0.0    19.0     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
0.0     0.0
```

TC, ... DIPOLE - Experimental values of these physical properties were not input:

```
0.0     0.0     0.0     0.0     0.0     0.0     0.0
```

AMCH3 - The number of CH_3 and CH_2 groups in acetic acid are input:

1.0

GCGB - The pertinent group index numbers from Table V., page 76 are input. After all the groups have been identified, the remaining data fields are filled by the end group index number 38.0.

```
2.0          3.0          1.0          38.0 ... 38.0
```

AMGB - The number of times the group identified in GCGB is present. When the end group index is input for GCGB, AMGB is 1.0.

```
1.0          1.0          1.0          1.0 ... 1.0
```

IXOT, IYOT - Input the index number corresponding to the functional group IXOT (Table VI, page 78) and the hydrocarbon radical type IYOT (Table VII, page 79).

```
        30               1
```

XN, XM,Q - Input the number of atoms, number of freely rotating bonds and the number of bonds in acetic acid respectively:

8.0 1.0 7.0

GCAMB - Input the index number corresponding to the groups listed in Table IV, page 70. After all the groups have been identified, the end group index number (58) is read in:

1.0 8.0 16.0 54.0 58.0 ... 58.0

CALC - All the physical properties will be estimated; thus CALC is 1.0.

ALIQ - Acetic acid is in the gas phase; the input is

0.0

APAC - Since CALC is 1.0 (all physical properties will be estimated) the input is all zeros.

AAC, BAC, CAC - Since the phase is known (ALIQ = 0.0, gas phase) the Antoine Cox constants are not needed; the input is

0.0 0.0 0.0

VISCPT, TTT - Since acetic acid is in the gas phase and this is the liquid viscosity, the input is

0.0 0.0

SURT PT, TTH - Since acetic acid is in the gas phase and this is the liquid phase surface tension, the input is

0.0 0.0

AADAT - Input the appropriate index numbers of the groups listed in Table VII, page 79. After all groups have been identified, fill the remaining data fields with 0.0.

```
1.0      16.0     41.0     93.0    124.0    128.0    130.0    131.0
145.0   146.0    147.0    170.0    171.0    180.0    201.0      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      0.0      0.0      0.0      0.0
```

<u>CADAT</u> - Input the number of times the group identified in AADAT is present in acetic acid. When AADAT is 0.0, the CADAT is also 0.0.

```
1.0      1.0      1.0      1.0      1.0      4.0      2.0      2.0
2.0      2.0      1.0      1.0      3.0      1.0      1.0      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      0.0      0.0      0.0      0.0
```

<u>PN</u> - Since only one pressure and temperature is being considered, PN is 1.0.

<u>T,P</u> - Input the temperature and pressure at which the physical properties of acetic acid will be estimated.

```
          375.0          0.50
```

RESULTS

Thirty-three compounds (organic - nonpolar and polar, inorganic - nonpolar and polar) were tested with and without the input of available experimental properties in the gas phase. Tables I and II contain a summary of the percent deviation for the various compound types where:

$$\% \text{ deviation} = \frac{(\text{calculated} - \text{experimental})}{\text{experimental}} \times 100$$

More accurate physical property estimations were possible when allowed available experimental data were used (28.75% vs 16.99% average error, for the gas phase) since all estimation techniques in level 2 or higher of R.C. Norris's levels (1) use other estimated physical properties (especially the experimental physical properties that can be input into the program). This pyramids the error of the higher level estimation techniques regardless of the accuracy of the method itself and explains the high % deviation without experimental input (28.75% for gas phase - 26.5% for the liquid phase).

Table IA summarizes the testing of seventeen organic compounds (with an experimental value input for viscosity) without experimental value input (critical properties, etc., were estimated in the gas program) for the liquid phase program.

Neither program should be used for inorganic compounds since the methods were all designed for organic compounds.

TABLE I

PERCENT DEVIATION WHEN NO EXPERIMENTAL INPUT USED

Numbers in ( ) indicate number of points used in average

Property	ORGANIC			INORGANIC	TOTAL ORGANIC AND INORGANIC
	Nonpolar	Polar	Total-Nonpolar & Polar	Total-Nonpolar & Polar	
Tb	12.03 (8)	3.39 (16)	6.26	39.68 (7)	13.81
Vb	8.37 (3)	9.15 (7)	8.92	115.15 (2)	26.62
Tc	11.22 (8)	3.38 (16)	5.99	39.98 (7)	13.67
Pc	2.92 (7)	5.52 (16)	4.71	34.86 (7)	11.76
Vc	10.97 (7)	10.31 (14)	10.51	47.15 (5)	17.57
Zc	2.97 (7)	9.42 (14)	7.26	9.59 (5)	7.69
VP	58.10 (1)	23.62 (12)	26.20		26.20
αc	3.07 (6)	1.44 (10)	2.06	4.99 (4)	2.64
ω	36.15 (7)	5.63 (4)	25.00	68.63 (3)	34.53
C_p°	2.67 (5)	3.23 (5)	2.95	5.38 (2)	3.35
ϵ/k	17.48 (4)	17.00 (5)	17.20	50.00 (7)	31.56
σ	6.28 (4)	7.00 (5)	6.69	24.06 (7)	14.28
b°	19.96 (4)	21.49 (5)	20.80	146.69 (7)	76.29
dipole	....	22.87 (13)	22.87	22.15 (1)	22.82
μ°	6.60 (6)	14.87 (5)	10.38	28.51 (6)	13.24
k	16.62 (3)		16.62	54.45 (4)	45.36
$\Delta H^\circ vb$	14.06 (6)	4.04 (13)	7.19	38.44 (7)	15.61
$\Delta H^\circ f$	14.22 (8)	16.53 (11)	15.55	39.17 (6)	21.22
ΔF_f°	69.08 (8)	46.28 (11)	55.88	120.16 (4)	67.06

TABLE IA

% DEVIATION WHEN NO EXPERIMENTAL PROPERTIES WERE USED*

LIQUID PROPERTIES

Numbers in () indicate number of points used in average

Property	Organic Nonpolar	 Polar	Total Polar and Nonpolar
C_p^o	19.42% (4)	24.18% (3)	21.5%
ρ	8.25% (5)	2.51% (5)	5.35%
μ	4.8% (3)	10.3% (5)	8.24%
Surface Tension	51.2% (3)	24.48% (5)	34.5%
Coeff. of Thermal Expansion	10.7% (2)	7.13% (4)	8.31%

* except viscosity

TABLE II

PERCENT DEVIATION WHEN EXPERIMENTAL INPUT IS USED

Numbers in ( ) indicate number of points used in average

Property	ORGANIC			INORGANIC	TOTAL ORGANIC AND INORGANIC
	Nonpolar	Polar	Total	Total Nonpolar & Polar	
VP	3.80 (1)	4.53 (12)	4.48	1.70 (1)	4.28
α_c	0.44 (6)	0.36 (10)	0.39	5.33 (6)	1.74
ω	9.00 (7)	5.02 (4)	7.56	7.92 (3)	7.63
C_p°	2.67 (5)	3.23 (5)	2.95	5.38 (2)	3.35
ϵ/k	9.23 (4)	27.26 (5)	19.24	22.21 (9)	20.73
σ	3.32 (4)	7.37 (5)	5.57	6.71 (9)	6.14
b°	9.43 (4)	19.13 (5)	14.82	22.55 (9)	8.68
μ°	7.51 (6)	9.74 (5)	8.52	15.51 (8)	11.47
k	9.07 (3)		9.07	53.01 (3)	31.04
ΔH°_{vb}	0.60 (6)	4.85 (13)	3.51	17.48 (9)	8.00
ΔH°_f	14.22 (8)	16.53 (11)	15.55	39.17 (6)	21.22
ΔF_f°	69.08 (8)	46.28 (11)	55.88	120.16 (4)	67.06

DISCUSSION AND RECOMMENDATIONS

This program was structured for ease of inserting improved estimation methods, since only poor estimations were available for some of the properties in both the gas and especially the liquid programs.

Presently, vapor pressure cannot be estimated accurately. The AIChE program concedes this fact and requires the vapor pressure to be input from either experimental data or an educated guess. Also there are no good estimation techniques for the potential parameters (gas program).

In general, the gas phase estimation techniques are advanced compated to the liquid phase methods. Only the recent techniques fitting analytical equations to the Lyderson, Greenkorn and Hougen charts are accurate, and they are the only methods employed in the AIChE program. In this work, poor estimation methods were used for isothermal heat capacity depa ture, isothermal entropy departure, viscosity and surface tension. The errors obtained by the program for the various estimation methods were found, in general, to be considerably greater than those claimed by their developers.

This program presently uses 90% of the working storage space available in a Spectra 70/45, 256K. Expansion will require the input of an overlay mapping program, which will severely lengthen the program running time. Another way of increasing the working storage would be to delete the structural input and require the user to input the value of the groups for each of the methods.

I recommend some revisions and additions for greater program flexibility and accuracy. These include:

- replacing the potential parameter estimation method with a more accurate technique when available;
- printing out a physical property when it is calculated as a debugging aid, since a program error terminates the program without a print-out;
- using an equation of state other than the Redlich-Kwong equation in the gas program;
- replacing the isothermal heat capacity departure, isothermal entropy departure, viscosity and surface tension methods with more accurate estimation techniques when available; and
- adding a mixture physical property estimation program to this program.

NOMENCLATURE

A, B, C, AO, BO, CO, GAMM, ALPH = Benedict, Webb, Rubien equation constants

AA = output logic parameter

AAC, BAC, CAC =Antoine-Cox equation constants

AADAT = array of particular groups from consolidated input

ABW = array of enthalpy and free-energy functions

ABWAE = array of absolute entropies

ABWSF = subroutine for determining entropy and free energy of formation by Anderson, Beyer, and Watson's method (21)

ACP = array of bond frequencies

ADAT = consolidated group array for internal use

ALIQ = logic parameter for path to correct phase calculation method

ALPHA = Riedel factor

ALTAL = subroutine for determining Riedel factor by alternate method (10)

AMCG = array of parachor contributions

AMCGC = internal array for parachor

AMCH3 = number of CH_3 and CH_2 groups

AMGB, AMS, AMBRD, AMRD, AMF, AMVD, AMBE, AMABW, AMB = arrays of the total amounts of particular groups

APA = logic parameter

APAC = array of specific properties that can be calculated separately

APARC = parachor

APP, BPP, CPP, AOPP, BOPP, COPP, ALPP, GAMPP = reduced Benedict, Webb, Rubien constants (37)

NOMENCLATURE

APRH = reduced pressure too high - output logic parameter

APRL = reduced pressure too low - output logic parameter

ATRH = reduced temperature too high -output logic parameter

ATRL = reduced temperature too low -output logic parameter

ATBAC = boiling point-°K at pressure P

AVB = array of additive - volume increments

BB = array of output logic parameters

BBB = array of Verma and Doraiswamy's group contributions

BCB, BCBE, BCBRD, BCF, BCRD, BCVD, GCLYD, GCS, ECABW = array of the number of each group for a given compound

BE = array of bond energies

BEHF = subroutine for determining heat of formation by bond energy method (19)

BKO = subroutine for determining low pressure thermal conductivity by Bromley's method (26)

BONDS = total number of bonds in the compound

BPARC = subroutine for parachor via McGowan additive method (31)

BRDCPO = subroutine for determining CPO by Bennewitz, Rossner, and Dobratz's method (17)

BVIS = viscosity via Thomas method (32)

BWRCP = subroutine for isothermal heat capacity departure via Benedict, Webb, Rubion equation (39) (37)

BWRENT = subroutine for isothermal entropy departure via Hirschfelder, Buehler, McGee and Sutton equation of state (31)

CADAT = array of total amount of particular groups

CALC = logic parameter

CBU = subroutine for determining high pressure viscosity by Coremans and Beenakker method (25)

CC = logic parameter

NOMENCLATURE

CHE301 = main program name

CIROT = array of characteristic internal-rotational contributions

CIV = array of collision integrals for viscosity

CODE = array of compound classifications

COFTE = coefficient of thermal expansion 1/°K

COTE = subroutine for coefficient of thermal expansion (33)

CP = heat capacity at constant pressure, cal/g mole-°K

CPO = ideal gas heat capacity, cal/g mole-°K

CV = heat capacity at constant volume, cal/g mole-°K

D = array of parameters allowing for the dipole moment

DELH = enthalpy deviation, cal/g mole

DELPR = reduced delta pressure indicating saturated or compressed liquid

DELS = entropy deviation, cal/g mole-°K

DELTA = low pressure viscosity parameter

DENS = density gms/cc

DENTA = entropy departure $S'_0 = S_0 + R\ln(P_0/P_c)$ where P_0 is a standard pressure

DIPOLE = dipole moment, debyes

DIS =intermolecular distance, angstroms

DW = subroutine for determining acentric factor by use of definition (9)

EDW = subroutine for determining acentric factor by Edmister's method (9)

EF = entropy of formation at 1 atm and 298°K, cal/g mole°K

ENGY = potential parameter ϵ_0/k, °K

ENTYA = subroutine for isothermal enthalpy deviation via Yen Alexander method (38)

EVB = entropy of vaporization at TB, cal/g mole- °K

NOMENCLATURE

FEF =free energy of formation at 1 atm and 298°K, kcal/g mole

FHF =subroutine for determining heat of formation by Franklin's method (20)

FRK =array of Franklin's group contributions

FUGCOF =fugacity coefficient

GB =array of Garcia-Barcena group contributions

GCGB, GCABW =array of group contribution indices

HF =heat of formation at T, kcal/g mole

HSV =hard-sphere volume b_o, cc/g mole

HTCAP =isothermal heat capacity cal/gm mole

HVB =heat of vaporization at TB, cal/g mole

IBCB, IBCBE, IBCBR, IBCF, IBCRD, IBCVD, IGCLY, IGCS, IECAB, IPARC =arrays indicating which of the consolidated group array are required for a particular method.

IXOT =functional group index

IYOT =hydrocarbon radical type index

JSTU1, JSTU2 =subroutine for determining high pressure viscosity by Jossi, Stiel, and Thodos method (24)

MALPHA =subroutine for determining Riedel factor by Miller's method (10)

N =number of compounds and conditions at which the program is to be used

NAME =compound name

NELE =number of different elements in compound

NO =number of different types of bonds in compound

P =pressure at which compound properties are desired

PART2 =second part of main program

PC =critical pressure, atm

NOMENCLATURE

PCLYD, TCLYD, VCLYD = arrays for Lydersen's group contributions

PN = number of pressure and temperature inputs for the same compound

PO1 = first of two output subroutines

PO2 = second of two output subroutines

PQ = array of functional groups

Q = number of bonds in molecule

RALPHA = subroutine for determining Riedel factor by Riedel's method (10)

RD = array of Rihani and Doraiswamy's group contributions

RDCPO = subroutine for determining CPO by Rihani and Doraiswamy's method (18)

RHOR = reduced density

RKCP = subroutine for determining CP by use of Redlich-Kwong equation of state

RKCV = subroutine for determining CV by use of Redlich-Kwong equation of state (28)

RKZ = subroutine for determining Z, V, H', S', and by use of Redlich-Kwong equation (2)

RPMVP = subroutine for determining vapor pressure by Riedel-Plank-Miller method (15)

SATL = internal parameter indicating if saturated or compressed liquid calculation was used

STK = subroutine for determining high pressure thermal conductivity by Stiel and Thodos method (27)

STLJP = subroutine for determining potential parameters by Stiel and Thodos method (27)

STUO1, STUO2, STUO3 = subroutines for determining low pressure viscosity by Stiel and Thodos method (23)

SURT = subroutine for surface tension via parachor method (34)

NOMENCLATURE

SURTE =surface tension dynes/cm

SURTPT =experimental liquid surface tension value at temperature TTTT

T =temperature at which compound properties are desired

TB =normal boiling point, ^{o}K

TBAC =subroutine for boiling point at pressure P via Antoine-Cox equation (35)

TC =critical temperature, ^{o}K

THC =high pressure thermal conductivity, cal/cm-sec-^{o}K

THEATA =TB/TC

TMUO1,TMUO2 =subroutines for determining low pressure viscosity by theoretical method (22)

TS =array of temperature increments of collision integrals

TT =array of temperature increments

TTT =temperature at which VISCPT is valid

TTTT =temperature at which SURTPT is valid

U =high pressure viscosity, centipoise

UO =low pressure viscosity, centipoise

V =volume, cc/g mole

VC =critical volume, cc/g mole

VD =array of Verma and Doraiswamy's group contributions

VDHF =subroutine for determining heat of formation by Verma and Doraiswamy's method (20)

VISCPT =experimental liquid viscosity value at temperature TTT in centipoise

VISC =liquid viscosity,centipoise

VP =vapor pressure, atm

NOMENCLATURE

W =acentric factor

WT =molecular weight of compound

XM =number of freely rotating bonds in compound

XN =number of atoms in compound

Y =array of hydrocarbon radical types

YWDEN =subroutine for density via Yen Woods method (36)

Z =compressibility factor

ZC =critical compressibility factor

ZZ =output logic parameter

Z1,Z2,Z3 =roots of the Redlich-Kwong equation of state

NOMENCLATURE

PART 2

BENVB = subroutine for determining VB by Benson's method (14)

GBZC = subroutine for determining ZC by additive technique (Garcia - Barcena) (7)

GLVC = subroutine for determining VC by use of gas law

GLZC = subroutine for determining ZC by use of gas law

LYDPC = subroutine for determining PC by Lydersens method (5)

LYDTB = subroutine for determining TB by Lydersen's method (11)

LYDTC = subroutine for determining TC by Lydersen's method (4)

LYDTH = subroutine for determining THEATA by Lydersen's method (4)

LYDVC = subroutine for determining VC by Lydersen's method (8)

LZC = subroutine for determining ZC by Lydersen's method (6)

OTTB = subroutine for determining TB by Ogata and Tsuchida method (12)

RPMHS = subroutine for determining enthalpy and entropy of vaporization by Riedel-Plank-Miller equation (16)

SVB = subroutine for determining VB by Schroeder's method (14)

WATTB = subroutine for determining TB by Watson's method (11)

X = logic parameter

TABLE III
CODE
COMPOUND CLASSIFICATION

CLASS	INDEX (I)
Monoatomic	1
Linear	2
Nonlinear	3
Polar--hydrogen bonding	4
Polar--non-hydrogen bonding	5
Nonpolar	6
Inorganic	7
Simple molecule if more than one funct'l group(R in Table VI) then	8
Complex molecule it is a complex molecule	9
Low boiling "permanent" gas	10
More than one functional group	11
Halogenated	12
Aliphatic halide	13
Conjugated	14
Contains triple bonds	15
Ester	16
Anhydride	17
Nitrile	18
Acid	19
Ketone	20
Alcohol	21
Thioether	22

TABLE III (Cont.)

CLASS	INDEX (I)
Has other than chlorine derivatives	23
Substituted acetylene	24
Phenol	25
Aniline	26
H_2	27
Br_2	28
F_2	29
I_2	30
He	31
H_2O	32
NH_3	33
Hydrocarbon	34

TABLE IV

Input for Determining Entropy and Free Energy of Formation Via Anderson, Beyer, and Watson's Method

GCABW

GROUP	INDEX (I)
Base-group Contributions:	
Methane	1
Cyclopentane	2
Benzene	3
Naphthalene	4
Methylamine	5
Dimethylamine	6
Dimethyl ether	7
Contributions of Primary CH_3 Substitution Groups:	
Methane	8
Cyclopentane:	
a. First-substitution outside ring	9
b. Enlargement of ring	10
Benzene and naphthalene:	
a. First-substitution outside ring	11
b. Second substitution:	
Ortho	12
Meta	13
Para	14
c. Third substitution (sym)	15

GROUP			INDEX (I)
Secondary Methyl Substitutions:			
A		B	
1		1	16
1		2	17
1		3	18
1		4	19
1		5	20
2		1	21
2		2	22
2		3	23
2		4	24
2		5	25
3		1	26
3		2	27
3		3	28
3		4	29
3		5	30
1	-O- in ester or ether		31
Substitution of H of OH group to form ester			32
Multiple-bond Contributions:			
A	Type of bond	B	
1	=	1	33
1	=	2	34

GROUP			INDEX (I)
Multiple-bond Contributions (Continued):			
A	Type of bond	B	
1	=	3	35
2	=	2	36
2	=(cis)	2	37
2	=(trans)	2	38
2	=	3	39
Corrections for each pair of conjugated double bonds			40
1	≡	1	41
1	≡	2	42
2	≡	2	43
Correction for double bond adjacent to aromatic ring			44
Substition of CH_3 by Nonhydrocarbon Groups:			
-OH (aliphatic, meta, para)			45
$-NO_2$			46
-CN			47
-Cl			48
-Br			49
-F			50
-I			51
=O (aldehyde)			52
=O (ketone)			53
-COOH			54

GROUP	INDEX (I)
Substitution of CH_3 by Nonhydrocarbon Groups (Continued):	
$-SH$	55
$-C_6H_5$	56
$-NH_2$	57
End	58

Instructions for Table IV

Each compound is considered to be composed of a basic group which has been modified by the addition of other groups. The base groups are indes numbers 1-7 and are either present or not (either 1.0 or 0.0). For example, ethanol is a modification of methane, ie, methane with a methyl substitution for one hydrogen. The first substitution of a methyl group for a hydrogen on a base group is called a primary methyl substitution. Any further substitution by CH_3, either for a hydrogen on the basic group or for a hydrogen on the primary substitution group is termed a secondary methyl substitution. The increment to be added here depends both upon the types of atoms adjacent to the substituted atom and upon the type of carbon atom upon which the substitution is made. The letter A is the carbon atom upon which the substitution is made and the letter B the highest tupe number (see below) of a carbon atom adjacent to A. The type numbers are as follows:

TYPE	
1	CH_3
2	CH_2
3	CH
4	C
5	C(in benzene or naphthalene ring)

Thus a substitution of a hydrogen in ethane by CH_3 to form propane would be a secondary methyl substitution and would be denoted as a 1,1 type of substitution since A=1, B=1. A secondary methyl substitution of a hydrogen in toluene to form ethyl benzene would be a type A=1, B=5 or 1,5.

Two special secondary substitutions are defined; one is used in forming a methyl ester from a carboxylic acid and the other in forming ethyl ester or ether from a methyl ester or ether. Contributions for multiple bonds and for nonhydrocarbon groups are also included. The latter group contributions, when added, are substituted for a methyl group, not a hydrogen atom.

TABLE V

Input for Determining ZC by Additive Technique (Garcia - Barcena)

GCGB

STRUCTURE	INDEX (I)
-H	1
$-CH_3$ of $-CH_2-$:	
First 10 in molecule	2
Each after the tenth	3
$-\overset{/}{C}H-$ of $-\overset{/}{\underset{\mid}{C}}-$:	
First in molecule	4
Each successive one	5
-CH in ring	6
Ring closure:	
3-membered ring	7
5-membered ring	8
6-membered ring	9
Benzene ring	
(including atoms and bonds)	10
Substitutional forms:	
Ortho	11
Meta	12
Para	13
1,2,3	14
1,2,4	15
1,3,5	16
C=C bond:	
First	17
Second	18

STRUCTURE	INDEX (I)
Isomerism:	
Cis	19
Trans	20
$C\equiv C$	21
$-NH_2$:	
Aliphatic	22
Aromatic	23
$-NH-$ aliphatic	24
$>N-$ aliphatic	25
$-SH$	26
$-S-$	27
$-O-$	28
$-O-$ ring	29
$HCOO-$ (formates):	
4 carbon atoms or less	30
More than 4 carbon atoms	31
$-COO$ (esters):	
5 carbon atoms or less	32
More than 5 carbon atoms	33
$-F$ (aromatic)	34
$-Cl$ (aromatic)	35
$-Br$ (aromatic)	36
$-I$ (aromatic)	37
End	38

TABLE VI

Input for TB by Ogata and Tsuchida Method

IKCT

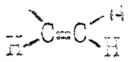
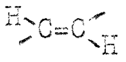
STRUCTURE	INDEX (I)	STRUCTURE	INDEX (I)
RH	1	HCOR	21
RCl	2	MeCOR	22
RBr	3	EtCOR	23
RI	4	RCN	24
ROH	5	RCOCl	25
MeOR	6	HCOOR	26
EtOR	7	MeCOOR	27
ROR	8	EtCOOR	28
PhOR	9	PhCOOR	29
$RONO_2$	10	RCOOH	30
RSH	11	RCOOMe	31
RSMe	12	RCOOEt	32
RSEt	13	RCOOPr	33
RSR	14	RCOOPh	34
RNH_2	15	$(RCO)_2O$	35
RNHMe	16	$ClCH_2COOR$	36
RNHEt	17	$Cl_2CHCOOR$	37
RNHPr	18	$BrCH_2COOR$	38
$RNMe_2$	19	$NCCH_2COOR$	39
RNO_2	20	$CH_2{=}CHCOOR$	40

TABLE VIII
Input for TB by Ogata and Tsuchida Method
IYOT

STRUCTURE	INDEX (I)
Methyl	1
Ethyl	2
n-Propyl	3
Isopropyl	4
n-Butyl	5
sec-Butyl	6
Isobutyl	7
t-Butyl	8
n-Pentyl	9
Isopentyl	10
t-Pentyl	11
Neopentyl	12
n-Hexyl	13
Isohexyl	14
n-Heptyl	15
n-Octyl	16
Vinyl	17
Allyl	18
2-Butenyl	19
Phenyl	20

TABLE VIII
Consolidated Group Input Table
AADAT

GROUP		INDEX No.
$-CH_3$		1
$>CH_2$		2
$\geq CH$		3
$-\overset{\vert}{\underset{\vert}{C}}-$		4
$>C=$	not including $C\genfrac{}{}{0pt}{}{=O}{-OH}$	5
$=\overset{\vert}{C}H$	not including $C\genfrac{}{}{0pt}{}{=O}{-OH}$	6
$=CH_2$		7
$=C=$		8
$\equiv CH$		9
$\equiv C-$		10
$-C\equiv N$		11
$-N\equiv C$		12
$-N=C$		13
$\genfrac{}{}{0pt}{}{H}{>}C=O$		14
$>C=O$	not including $C\genfrac{}{}{0pt}{}{=O}{-OH}$	15
$-C\genfrac{}{}{0pt}{}{=O}{-OH}$		16
$-C\genfrac{}{}{0pt}{}{O-}{=O}$	not including $C\genfrac{}{}{0pt}{}{=O}{-OH}$	17
$\begin{array}{l}-C\genfrac{}{}{0pt}{}{=O}{-O}\\-C\genfrac{}{}{0pt}{}{/}{=O}\end{array}$		18
$-NH_2$		19
$>NH$		20
$-\overset{\vert}{N}-$		21
$-NO_2$		22
$-ONO$		23
$-ONO_2$		24

GROUP	INDEX
N≡ aliphatic	25
=NH aliphatic	26
$-NO_2$ aliphatic	27
–SH	28
–S–	29
$-SO_3H$	30
=S	31
SH rhombic crystal	32
–S– rhombic crystal std. state	33
–O– ether	34
–O– from GCLYD and BCVD (not –OH)	35
=O other from GCLYD	36
–O– ring	37
–OH primary	38
–OH secondary	39
–OH tertiary	40
–OH all	41
–F	42
–Cl	43
–Br	44
–I	45
	46
 trans	47

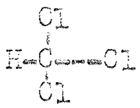
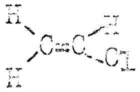
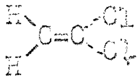
GROUP	INDEX
$_{H}{>}C{=}C{<}_{H}$ cis	48
$>C{=}C{<}^{H}_{H}$	49
$>C{=}CH_2$	50
$>C{=}C{<}_{H}$	51
$>C{=}C{<}$	52
$^{H}{>}C{=}C{=}CH_2$	53
$>C{=}C{=}CH_2$	54
$^{H}{>}C{=}C{=}C{<}^{H}$	55
CH_3-OH	56
$HO-\overset{\mid}{\underset{\mid}{C}}-H$	57
$-\overset{\mid}{\underset{\mid}{C}}\ -OH$	58
$-CH_2-OH$ from BKO internal rotation	59
$-OH$ phenol	60
$-\overset{\mid}{C}H_2$ ring	61
$-\overset{\mid}{C}H-$ ring	62
$-\overset{\mid}{\underset{\mid}{C}}-$ ring	63
$>C=$ ring	64
$=\overset{/}{C}H$ ring	65
$=C=$ ring	66
$>C{=}O$ ring	67
$>NH$ ring	68
$>N-$ ring	69
$-S-$ ring	70
$-NH_2$ aromatic	71
$=NH$ aromatic	72
$\equiv N$ aromatic	73

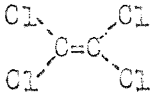
GROUP	INDEX
C_6 cycloparaffin ring	74
C_5 cycloparaffin ring	75
C_4 cycloparaffin ring	76
C_3 cycloparaffin ring	77
3 membered ring	78
4 membered ring	79
5 membered ring	
pentane	80
pentene	81
6 membered ring	
hexand	82
hexene	83
$-CH_2-CH_2$ from BKO internal rotation	84
CH_3-CH_2- from BKO	85
$R-\overset{\vert}{\underset{\vert}{C}}-H$ from BKO	86
$R-\overset{\vert}{\underset{\vert}{C}}-$ from B KO	87
$R-CH=$ (TYPE Va) from BKO	88
$R-CH=$ (TYPE Vb) from BKO	89
$=CH-CH=$ from BKO	90
$\equiv C-C\equiv$ from BKO	91
$R-\overset{\vert}{C}=$ from BKO	92
$CH_3-\overset{R}{C}=O$ from BKO	93
$RCH_2-O-RCH_2$ from BKO	94

NOTE: choose bonds as similar as possible to the bonds in the compound for the BKO contributions

GROUP	INDEX
$\overset{\leftrightarrow}{\leftrightarrow}{>}CH$	95
$\overset{\leftrightarrow}{\leftrightarrow}{>}C\leftrightarrow$	96
$\overset{\leftrightarrow}{\leftrightarrow}{>}C\leftrightarrow$	97
$\leftrightarrow CH_2$	98
$\leftrightarrow C{<}^{H}$	99
$\leftrightarrow NH_2$	100
$\leftrightarrow S\leftrightarrow$	101
$\leftrightarrow N\leftrightarrow$	102
$O{<}^{\leftrightarrow}_{\leftrightarrow}$	103
$HO-C{<}^{\leftrightarrow}_{\leftrightarrow}$	104
quaternary C not adjacent to terminal methyl(paraffin chain)	105
1,2 Dimethyl or 1,3 methyl ethyl (correction for aromatic substitution)	106
1,2 Methyl ethyl or 1,2,3 trimethyl (correction for aromatic substitution)	107
$-CH_2-OH$ from BCVD	108
double bond between carbon atoms	109
triple bond between carbon atoms	110
ethyl side chain (paraffin)	111
3 adjacent CH groups (paraffin)	112
adjacent C and CH groups (paraffin)	113
adjacent quaternary C (paraffin)	114
side chain with 2 or more C atoms	115
Benzene from BEHF	116
Naphthalene from BEHF	117

NOTE: BEHF is structure type only and is either 1 or 0

GROUP	INDEX
Aniline from BEHF	118
Dialkyl Carbonate from BEHF	119
Furfural from BEHF	120
Phenyl acetylene from BEHF	121
Phenyl cyanide from BEHF	122
Aceto phenone from BEHF	123
Methane from BEHF	124
Methyl amine from BEHF	125
Dimethyl amine from BEHF	126
Dimethyl Ether from BEHF	127
Hydrogen	128
Nitrogen	129
Carbon	130
Oxygen	131
Sulfur	132
Anthracene	133
$Cl—CH_3$	134
$Cl—CH_2—CH_3$	135
 $H_3C—\overset{H}{\underset{Cl}{C}}—Cl$	136
	137
 $H—\overset{Cl}{\underset{Cl}{C}}—Cl$	138
 $Cl—\overset{Cl}{\underset{Cl}{C}}—Cl$	139
	140
	141

GROUP	INDEX
 cis 1,2	142
 trans 1,2	143
	144
$H_2(g) \rightarrow 2H(g)$	145
$C(graphite) \rightarrow C(g)$	146
$O_2(g) \rightarrow 2O(g)$	147
$F_2(g) \rightarrow 2F(g)$	148
$Cl_2(g) \rightarrow 2Cl(g)$	149
$Br_2(g) \rightarrow 2Br(g)$	150
$I_2(c) \rightarrow I_2(g)$	151
$I_2(g) \rightarrow 2I(g)$	152
$S(c) \rightarrow S(g)$	153
$N_2(g) \rightarrow 2N(g)$	154
S as S ideal gas	155
S as S_2 ideal gas	156
P_2 ideal gas	157
$-CH_3^{\circ}$	158
$>\overset{\circ}{C}H$	159
$-\overset{\vert}{\underset{\vert}{C}}{}^{\circ}$	160
$-\overset{\circ}{O}$	161
$-O-O_{\circ}$	162
$-S_{\circ}$	163
$-\overset{+}{C}H_2$	164

GROUP	INDEX
$>\overset{+}{C}H$	165
$-\overset{\mid}{\underset{\mid}{C}}+$	166
$-\overset{+}{C}=CH_2$	167
$-HC=\overset{+}{C}H$	168
$-S+$	169
C–C including resonating structures	170
C–H including resonating structures	171
C=C " " "	172
C≡C " " "	173
C–F " " "	174
C–Cl " " "	175
C–Brr " " "	176
C–I " " "	177
C–N " " "	178
C–S " " "	179
C–O " " "	180
C=O aldehydes including resonating structures	181
C=O ketones " " "	182
N–N	183
N≡N	184
N–H	185
S–H	186
S–S	187

GROUP		INDEX
C-O		188
N-O		189
C=S		190
N=O		191
C=O all		192
Single branching	6 membered rings cyclo paraffin	193
Double branching		
1,1		194
cis 1,2		195
trans 1,2		196
cis 1,3		197
trans 1,3		198
cis 1,4		199
trans 1,4		200
Single branching	5 membered rings cyclo paraffin	201
Double branching		
1,1		202
cis 1,2		203
trans 1,2		204
cis 1,3		205
trans 1,3		206
Double branching	Aromatics	
1,2		207
1,3		208
1,4		209
Triple branching		
1,2,3		210
1,2,4		211
1,3,5		212
S as RCNS		213
S as RSSR		214

TABLE IX
Input for the Estimation of Particular Physical Properties
APAC

Read in 1.0 if property is desired and 0.0 if not.

PROPERTY	INDEX
Acentric factor	1
Reidel factor	2
Lennord Jones parameters	3
Ideal gas $C_p - C_p\phi$	4
Heat of formation	5
Entropy and free energy of formation	6
Low pressure viscosity	7
High pressure viscosity	8
Low pressure thermal conductivity	9
High pressure thermal conductivity	10
Vapor pressure	11
DELH, DELS, FUGCOF, V, Z	12
C_p	13
C_v	14
LIQUID	
Density	15
Coefficient of thermal expansion	16
Parachor	17
Viscosity	18
Heat capacity departure	19
Isothermal enthalpy departure	20
Surface tension	21
Isothermal entropy deviation	22

```
      PROGRAM CHE301
      DIMENSION IBCB(216),IBCBE(216),IBCBR(216),IBCF(216),IBCRD(216),
     1IBCVD(216),IGCLY(216),IGCS(216),IFCAB(216)
      DIMENSION NAME(20),PCLYD(41),TCLYD(41),VCLYD
     1(41),ABWAE(14),AB%(58),CIRCT(9,12),ACP(20,6),
     2CIV(37,8),TS(37),D(8),RD(47,4),VD(50,2),
     3BBB(80,2),TT(9),FRK(65,9),RE(40),GB(38),PQ
     4(40,2),Y(20),AVB(18),RB(13),GCLYD(41),
     5GCBS(10),AMGP(10),GCS(17),BCBRD
     6(20),BCRD(46),BCF(64),
     7BCVD(80),VDM(80),BCBE(40),
     8GCABB(10),FCABB(13),BCB(12),
     9CBBF(34),APA(23,2),APAC(23)
      DIMENSION ADAT(216)
      DIMENSION AMCG(9),
     1APP(4),AOPP(4),BPP(4),BOPP(4),CPP(4),COPP(4),
     2ALPP(4),GAMPP(4),
     3AMCGC(9),IPARC(216)
      DIMENSION A(4,6),AOC(4),AWC(4),AQ(4),AW(4),
     1AT(4),AADAT(48),CADAT(48)
      READ 9000,(IBCB(I),I=1,216)
      READ 9000,(IBCBE(I),I=1,216)
      READ 9000,(IBCBR(I),I=1,216)
      READ 9000,(IBCF(I),I=1,216)
      READ 9000,(IBCRD(I),I=1,216)
      READ 9000,(IBCVD(I),I=1,216)
      READ 9000,(IGCLY(I),I=1,216)
      READ 9000,(IGCS(I),I=1,216)
      READ 9000,(IFCAB(I),I=1,216)
      READ 9000,(IPARC(I),I=1,216)
      READ          1019,(AMCGC(N),N=1,9)
      DO 8 I=1,4
    8 READ          2017,APP(I),AOPP(I),BPP(I),BOPP(I),CPP(I),COPP(I),
     1ALPP(I),GAMPP(I)
      READ          1019,((FRK(I,J),I=1,64),J=1,9)
      READ          1117,((RD(I,J),I=1,46),J=1,4)
      DO 5 I=1,79
    5 READ 1122,(VD(I,1),BBB(I,1),VD(I,2),BBB(I,2),VDM(I))
      DO 4 I=1,41
    4 READ          1002,TCLYD(I),PCLYD(I),VCLYD(I)
      READ          1023,(AVB(I),I=1,17)
      READ          1004,(ABWAE(I),I=1,13)
      READ          1012,((CIRCT(I,J),I=1,9),J=1,12)
      READ          1020,(RE(I),I=1,39).
      READ          1013,((ACP(I,J),I=1,20),J=1,6)
      READ          1014,((CIV(I,J),J=1,8),I=1,37)
      READ          1015,(TS(I),I=1,37)
      READ          1016,(D(I),I=1,8)
      READ          1011,(AB%(I),I=1,58)
      READ          1018,(TT(I),I=1,9)
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```
      READ        1021,(GH(I),I=1,38)
      READ        1022,((PQ(I,J),J=1,2),I=1,40)
      READ        1020,(Y(I),I=1,20)
      READ 1004,TC,PC,ZC,VC,TB,VB,DIPOLE
      READ 1013,V,Z,VP,ALPHA,W,CPO
      READ 1013,CP,CV,ENGY,DIS,HSV,UO
      READ 1013,U,THCO,DELH,DELS,FUGCOF
      READ 1013,HVB,EVB,HF298,HF,EF,FEF
      READ 1013,IHC
      READ 1013,DENS,DELH,HTCAP,VISC,VESND,APARC
      READ 1013,DENTA,SURTE,COFTE
      DO 8089 N=1,22
 8089 READ 8088,APA(N,1),APA(N,2)
      READ        1000,N
      DO 200 INDX=1,N
      READ        1001,(NAME(NN),NN=1,7)
      READ 1002,WT
      READ 8088,(CODE(LL),LL=1,34)
      NDCD=CODE(34)
      READ        1004,TC,PC,ZC,VC,TB,VB,DIPOLE
      READ        1081,ANCHB
      READ        1080,(GCHB(I),I=1,10)
      READ        1080,(AMGB(I),I=1,10)
      READ        1082,IXOT,IYOT
      READ        1002,XN,XM,Q
      READ        1080,(GCABW(I),I=1,10)
C     IF ALL PHYSICAL PROPERTIES ARE TO BE CALCULATED,
C     CALC=1.0, OTHERWISE CALC=0.0
      READ 1010,CALC
C     LIQUID PROGRAM IS CALLED IF ALIQ=1.0,IF 0.0,
C     VAPOR CALCULATION CONTINUES.  IF ALIQ=-1.0,
C     THE BOILING POINT IS CALCULATED AND THE
C     APPROPRIATE CALCULATION IS APPLIED
      READ 1010,ALIQ
C     IF A SPECIFIC PROPERTY IS TO BE CALCULATED
C     THEN APAC=1.0, IF NOT APAC=0.0
      READ 8088,(APAC(M),M=1,22)
C     READ ANTOINE COX CONSTANTS A,B AND C
      READ 1002,AAC,BAC,CAC
C     KNOWN LIQUID VISCOSITY POINT AT TEMPERATURE TTT
C     VISCOSITY IN CENTIPOISE AND TEMP. IN DEG K
      READ 2000,VISCPT,TTT
C     KNOWN LIQUID SURFACE TENSION POINT AT TEMP. TTTT
C     SURFACE TENSION IN DYNES/CM AND TEMP. IN DEG K
      READ 2000, SURTPT,TTTT
C     AADAT IS THE IDENTIFYING NUMBER OF A PARTICULAR
C     BOND OF THE 214 LISTED
      READ 3000, (AADAT(N),N=1,32)
C     CADAT IS THE NUMBER OF TIMES THE PARTICULAR BOND IS
C     PRESENT
```

```
      READ 3000, (CADAT(M),M=1,32)
      READ 1002,PN
      IPN=PN
      DO 200 I=1,IPN
      READ 1002,I,P
      ATRH=0.0
      ATRL=0.0
      APRL=0.0
      APRH=0.0
      SATL=0.0
      DO 3006 N=1,214
 3006 ADAT(N)=0.0
      DO 3001 M=1,32
      IF(AADAT(M)) 3007,3005,3007
 3007 DO 3001 N=1,214
      IF(N-AADAT(M)) 3001,3003,3001
 3003 ADAT(N)=CADAT(M)
 3001 CONTINUE
 3005 CONTINUE
C     END PART I
      IF(ALIQ) 797,798,799
  799 IF(CALC) 820,810,820
  820 DO 796 N=1,14
  796 APAC(N)=0.0
      DO 830 N=15,22
  830 APAC(N)=1.0
      GO TO 870
  810 DO 811 N=1,14
  811 APAC(N)=0.0
      GO TO 870
  798 IF(CALC) 840,850,840
  840 DO 841 N=1,14
  841 APAC(N)=1.0
      DO 842 N-15,22
  842 APAC(N)=0.0
      GO TO 870
  850 DO 851 N=15,22
  851 APAC(N)=0.0
      GO TO 870
  797 CALL TBACA (P,AAC,BAC,CAC,TBAC)
      IF(TBAC-T) 796,798,799
  880 CONTINUE
  870 DO 9557 L=1,15
 9550 DO 9557 N=1,22
      IF(APAC(N)) 9557,9557,9553
 9553 DO 9554 M=1,2
      IF(APA(N,M)) 9554,9554,9556
 9556 I=APA(N,M)
      APAC(I)=1.0
 9554 CONTINUE
```

```
 9557 CONTINUE
      L2=1.0
      M=1.0
      N=1.0
      M1=1.0
      M2=1.0
      M3=1.0
      M4=1.0
      M5=1.0
      M6=1.0
      M7=1.0
      DO 4000 I=1,214
      IF(IBCB(I)) 4001,4002,4001
 4001 BCB(M)=ADAT(I)
      M=M+1.0
 4002 IF(IBCHE(I)) 4003,4004,4003
 4003 BCHE(N)=ADAT(I)
      N=N+1.0
 4004 IF(IBCOR(I)) 4005,4006,4005
 4005 BCORO(M1)=ADAT(I)
      M1=M1+1.0
 4006 IF(IBCF(I)) 4007,4008,4007
 4007 BCF(M2)=ADAT(I)
      M2=M2+1.0
 4008 IF(IBCRD(I)) 4009,4010,4009
 4009 BCRD(M3)=ADAT(I)
      M3=M3+1
 4010 IF(IBCVD(I)) 4011,4012,4011
 4011 BCVD(M4)=ADAT(I)
      M4=M4+1.0
 4012 IF(IGCLY(I)) 4013,4014,4013
 4013 GCLYD(M5)=ADAT(I)
      M5=M5+1
 4014 IF(IGCS(I)) 4015,4016,4015
 4015 GCS(M6)=ADAT(I)
      M6=M6+1.0
 4016 IF(IECAB(I)) 4017,4018,4017
 4017 ECABW(M7)=ADAT(I)
      M7=M7+1.0
 4018 CONTINUE
 5001 IF(IPARC(I)) 5002,5005,5002
 5002 AMCG(L2)=ADAT(I)
      L2=L2+1.0
 5005 CONTINUE
 4000 CONTINUE
      DO 6 J=1,13
 6    BA(J)=0.
      AA=0.
      CALL    PART2 (PC,WT,TPCATA,TC,ZC,VC,VB,TB,HVB,CVB,
     1CODE,IXOT,IYOT,AMCHB,PCLYD,GCLYD,TCLYD,AVB,
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```
     2GCS,PO,Y,VCLYO,GP,GCOP,AMGB)
2222 IF(CODE(7)-7.)66,67,66
66   IF(CODE(21)-21.)68,67,68
68   IF(CODE(24)-24.)69,67,69
67   IF(CODE(15)-15.)70,71,70
71   BB(1)=1.
  69 CONTINUE
     IF(APAC(4)) 6000,6000,7000
7000 CALL RDCPD (BD,T,CPD,BCRD)
6000 GO TO 180
  70 CONTINUE
     IF(APAC(4)) 180,180,7001
7001 CALL BRDCPD (ACP,T,CPD,XN,XM,Q,BCBRD)
180  IF(CODE(12)-12.)72,73,72
  72 CONTINUE
     IF(APAC(5)) 6001,6001,7002
7002 CALL FHF (IT,FRK,T,HF,876,BCF,HF298)
6001 GO TO 74
73   IF(CODE(16)-16.)75,76,75
75   IF(CODE(17)-17.)77,76,77
77   IF(CODE(14)-14.)79,76,79
79   IF(CODE(23)-23.)80,78,80
  80 CONTINUE
     IF(APAC(5)) 6002,6002,7003
7003 CALL VDHF (T,VD,HF,BBP,876,BCVD,VDM,HF298)
6002 GO TO 74
78   IF(T-298.)76,82,76
82   IF(CODE(19)-19.)83,76,83
  83 CONTINUE
     IF(APAC(5)) 6003,6003,7004
7004 CALL BEHF (BE,HF,BCBE,HF298)
6003 GO TO 74
76   BB(12)=12.
  74 CONTINUE
     IF(APAC(6)) 87,87,7005
7005 CALL ABWSF (T,AB,AE,ABW,EF,FEF,GCABW,ECABW,HF298)
87   TBR=TB/TC
     IF(TBR-0.35)88,89,89
89   IF(TBR-1.00)90,88,88
  90 CONTINUE
     IF(APAC(2)) 6004,6004,7006
7006 CALL RALPHA (TB,TC,PC,ALPHA)
6004 GO TO 91
88   IF(CODE(25)-25.)92,93,92
  93 CONTINUE
     IF(APAC(1)) 6005,6005,7007
7007 CALL FDW (PC,THEATA,W)
6005 CONTINUE
     IF(APAC(2)) 6006,6006,7008
7008 CALL ALTAL (W,ALPHA)
```

```
6006 GO TO 3333
92   IF(CODE(26)-26.)95,93,95
95   IF(CODE(32)-32.)96,93,96
96   IF(CODE(28)-28.)97,93,97
  97 CONTINUE
     IF(APAC(2)) 91,91,7009
7009 CALL MALPHA (PC,THEATA,ALPHA)
91   IF(CODE(12)-12.)98,99,98
98   IF(CODE(16)-16.)100,99,100
 100 CONTINUE
     IF(APAC(1)) 6007,6007,7010
7010 CALL DW (TC,PC,TB,ALPHA,W)
6007 GO TO 3333
99   IF(CODE(15)-15.)101,100,101
101  IF(CODE(21)-21.)102,100,102
102  IF(CODE(14)-14.)103,100,103
 103 CONTINUE
     IF(APAC(1)) 3333,3333,7011
7011 CALL EDW (PC,THEATA,W)
C    END PART III
3333 IF(CODE(6)-6.)191,105,105
191  IF(DIPOLE)104,106,104
104  RB(2)=2.
     GO TO 105
106  DIPOLE=1.44
     GO TO 104
 105 CONTINUE
     IF(APAC(3)) 107,107,7012
7012 CALL STEUP (TC,ZC,PC,ENGY,DIS,HSV,VC,CODE(6),CODE
    1(4))
107  CALL RKZ (T,P,Z,B123,V,DELH,DELS,FUGCOF,Z1,Z2,Z3,
    1TC,PC)
     GO TO 124
123  AA=1.
     GO TO 190
 124 CONTINUE
     IF(APAC(11)) 6050,6050,7014
7014 CALL RPMVP (TB,TC,PC,T,ALPHA,VP)
6050 CONTINUE
     CC=0.
     IF(CODE(33)-33.)108,126,108
108  IF(CODE(6)-6.)131,132,132
 131 CONTINUE
     IF(APAC(7)) 6010,6010,7015
7015 CALL THU2 (T,WT,ENGY,DIS,CIV,TS,D,DIPOLE,DD,B133,
    1B134,B135,DELTA)
6010 GO TO 111
133  RB(3)=3.
     GO TO 135
134  RB(4)=4.
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            GO TO 136
      135   BB(5)=5.
            GO TO 138
       132 CONTINUE
            IF(APAC(7)) 6011,6011,7016
      7016 CALL THU01 (T,WT,ENGY,DIS,UD)
      6011 GO TO 111
      125   BB(6)=6.
            IF(CC-1.)136,137,137
      136   CC=1.
            GO TO 109
      137   BB(7)=7.
            GO TO 114
      138   IF(CC-1.)139,137,137
      139   CC=1.
            GO TO 127
      108   IF(CODE(19)-19.)109,126,109
      126   IF(CODE(6)-6.)127,110,110
      127   IF(CODE(5)-5.)128,129,110
      128   IF(CODE(4)-4.)110,130,110
       110 CONTINUE
            IF(APAC(7)) 6012,6012,7017
      7017 CALL STU01 (T,WT,TC,PC,ZC,UD,&125,RHOR)
      6012 GO TO 111
       129 CONTINUE
            IF(APAC(7)) 6013,6013,7018
      7018 CALL STU03 (T,WT,TC,PC,ZC,UD,&125,RHOR)
      6013 GO TO 111
       130 CONTINUE
            IF(APAC(7)) 111,111,7019
      7019 CALL STU02 (T,WT,TC,PC,ZC,UD,&125,RHOR)
       111 IF(CODE(8)-8.)112,113,112
       112 IF(CODE(6)-6.0) 140,141,141
       141 CONTINUE
            IF(APAC(8)) 6014,6014,7020
      7020 CALL JST01 (TC,PC,VC,V,UD,WT,U,&142,RHOR)
      6014 GO TO 114
      113   IF(CODE(6)-6.)140,181,140
       181 CONTINUE
            IF(APAC(8)) 6015,6015,7021
      7021 CALL CSU (T,UD,V,ENGY,HSV,U)
      6015 GO TO 114
       140 CONTINUE
            IF(APAC(8)) 6016,6016,7022
      7022 CALL JST02 (TC,PC,VC,V,UD,WT,U,&142,RHOR)
      6016 GO TO 114
      142   BB(8)=8.
       114 CONTINUE
            IF(APAC(13)) 6017,6017,7023
      7023 CALL RKCP (T,V,TC,PC,CPO,CP)
```

```
6017 CONTINUE
C        END PART IV
         IF(APAC(14)) 6019,6019,7024
7024 CALL RKCV (T,V,TC,PC,VC,CP,CV)
6019 CONTINUE
         IF(APAC(9)) 6051,6051,7025
7025 CALL BKO (T,WT,TC,VB,TB,U,CV,CODE1,CODE2,
        1SVS,CIRUG,THCO,RCF)
6051 CONTINUE
         IF(CODE(4)-4.)115,116,115
116      BB(11)=11.
         GO TO 122
115      IF(CODE(5)-5.)117,116,117
117      IF(CODE(27)-27.)118,116,118
118      IF(CODE(31)-31.)119,116,119
119      IF(PC-P)120,120,121
120      BB(10)=10.
         GO TO 122
 121 CONTINUE
         IF(APAC(10)) 6020,6020,7026
7026 CALL STK (ZC,TC,PC,V,WT,THCO,&162,THC,RHOR)
6020 GO TO 122
162      BB(9)=9.
C        END PART V
122      CONTINUE
190      CALL PO1 (PC,ZC,VC,VB,TB,TC,T,P,WT,NAME,BB,CPO,
        1ALPHA,W,Z1,Z2,Z3,VP,CP,CV,AA,V,Z,ZZ,&201)
         CALL PO2 (HVB,EVBSMI,HF,HCF,ENGY,DIS,HSV,DELH,
        1DELS,FUGCOF,OH,DELTA,RHOR,U,THCO,THC,AA,DIPOLE,
        2GB,T,P,ZL,HF298)
 201 CONTINUE
         IF(APAC(15)) 2900,2900,2901
2901 CALL YADEN(ZC,TC,T,VC,P,PC,DENS,DELPR,WT)
2900 IF(APAC(16)) 2902,2902,2903
2903 CALL COTE (TC,COFTE,T)
2902 IF(APAC(17)) 2904,2904,2905
2905 CALL APARC(ANCG,ANCGC,APARC,BONDS)
2904 IF(APAC(18)) 2906,2906,2907
2907 CALL JVIS (DENS,TC,TIT,VISCPT,T,ZC,VC,P,PC,WT,VISC)
2906 IF(APAC(19)) 2908,2908,2909
2909 CALL BWRCP (T,DENS,A,B,C,AO,BO,CO,RTCAP,ALPH,GAMM,
        1APP,BPP,CPP,AOPP,BOPP,COPP,ALPP,GAMPP,W,TC,PC,P,
        2GOLD,WT)
2908 IF(APAC(20)) 2910,2910,2911
2911 CALL ENTYA (T,P,DENS,PC,TC,VC,ZC,WT,DELH,DELPR,
        1ATCO,ATRL,APRH,APRL,SATL)
2910 IF(APAC(21)) 2914,2914,2915
2915 CALL SURT (APARC,DENS,WT,TB,SURTE,T,TC,SURTPT,TITT)
2914 IF(APAC(22)) 2916,2916,2917
2917 CALL BARENT (P,PC,T,TC,VC,DELTA,DELH,
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```
      1PT,DENS,ALPHA,ZC)
2916  CONTINUE
       CALL PUR (DENS,DFLH,HTCAP,VISC,VESHD,WT,
      1APARC,DELTA,SURTE,COFTE,T,P,PC,TC,VC,
      2ATKH,ATKL,APKH,APKL,SATL)
200   CONTINUE
2000  FORMAT (8F10.4)
2017  FORMAT (4F15.8/4F15.8)
3000  FORMAT (8F10.2)
   1  FORMAT (2F5.1,9F4.1,2F4.1)
1010  FORMAT (F10.3)
1011  FORMAT (2F10.3)
1012  FORMAT (12F6.2)
1013  FORMAT (6F10.3)
1014  FORMAT (8F8.4)
1015  FORMAT (F8.1)
1016  FORMAT (4F6.2)
1017  FORMAT (4F10.6)
1018  FORMAT (F10.1)
1019  FORMAT (9F6.2)
1020  FORMAT (5F10.1)
1021  FORMAT (F10.4)
1022  FORMAT (4F10.3)
1023  FORMAT (6F10.1)
1001  FORMAT (7A4)
1060  FORMAT (10F7.1)
1004  FORMAT (7F10.3)
1031  FORMAT (F10.3)
1083  FORMAT (15F4.1)
1003  FORMAT (F10.1)
1000  FORMAT (I5)
1002  FORMAT (5F10.3)
1032  FORMAT (2I5)
1117  FORMAT (5F10.5)
1122  FORMAT (5F10.3)
8088  FORMAT (6F10.3)
9000  FORMAT (16I2,9I2,10I2)
      STOP
      END
```

```
            SUBROUTINE PART2 (PC,WT,THEATA,TC,ZC,VC,VB,TB,HVB,EVB,
           1CODE,IXOUT,IYOUT,AMCH3,PCLYD,GCLYD,TCLYD,AVB,
           2GCS,PO,Y,VCLYD,GB,GCGB,AMGB)
            DIMENSION PCLYD(41),GCLYD(41),TCLYD
           1(41),CODE(33),AVB(16),GCS(17),PO
           2(40,2),Y(20),VCLYD(41),GB(38),GCGB(10),AMGB(10)
            IF(PC-0.)10,10,11
        10 CALL LYDPC (PCLYD,WT,PC,GCLYD)
        11 CALL  LYDTH (TCLYD,THEATA,GCLYD)
            IF(TC-0.)12,12,13
   13       IF(ZC-0.)14,14,15
   15       X=0.
            IF(VC-0.)16,16,17
   16       CALL GLVC (PC,TC,ZC,VC)
   17       IF(VB-0.)18,18,19
   18       IF(CODE(10)-10.)20,21,20
         21 CALL  SVB (AVB,VB,GCS)
            GO TO 19
   20       IF(CODE(18)-18.)22,21,22
   22       CALL SFNVB (VC,PC,VB)
   19       IF(X-0.)50,50,51
   50       IF(TB-0.)23,23,24
   23       IF(CODE(11)-11.)25,26,25
   26       CALL WATTB (THEATA,VB,TB)
            GO TO 24
   25       CALL BTTB (PO,Y,TB,IXOUT,IYOUT)
   24       CALL RPHUS (PC,TC,TB,HVB,EVB)
            GO TO 2222
   14       IF(TB-0.)27,27,28
   27       IF(CODE(11)-11.)29,30,29
   29       CALL BTTB (PO,Y,TB,IXOUT,IYOUT)
            GO TO 28
   30       CALL LYDTB (THEATA,TC,TB)
   28       IF(VC-0.)31,31,32
   32       CALL GLZC (PC,TC,VC,ZC)
            X=1.
            GO TO 17
         31 CALL  LYDVC (VCLYD,VC,GCLYD)
            CALL GLZC (PC,TC,VC,ZC)
            X=1.
            GO TO 17
   51       CALL RPHUS (PC,TC,TB,HVB,EVB)
            GO TO 2222
   12       IF(TB-0.)33,33,34
   33       IF(CODE(11)-11.)35,36,35
   35       CALL BTTB (PO,Y,TC,IXOUT,IYOUT)
   34       CALL LYDTC (TB,THEATA,TC)
            GO TO 43
   36       IF(VB-0.)37,37,38
   37       IF(VC-0.)39,39,40
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```
   39 CALL  SVB (AVB,VB,GCS)
      GO TO 38
 40   IF(CODE(10)-10.)41,39,41
 41   IF(CODE(18)-18.)42,39,42
 42   CALL RENVB (VC,PC,VB)
 38   CALL RATIB (THEATA,VB,TB)
      CALL LYDIC (TB,THEATA,IC)
 43   IF(VC-0.)44,44,45
 45   IF(ZC-0.)46,46,47
 46   CALL GLZC (PC,TC,VC,ZC)
      GO TO 47
 44   IF(ZC-0.)48,48,49
 49   CALL GLVC (PC,TC,ZC,VC)
      GO TO 47
 48   IF(CODE(13)-13.)52,53,52
 52   IF(CODE(4)-4.)54,53,54
 54   IF(CODE(5)-5.)55,53,55
 55   IF(CODE(7)-7.)56,53,56
 56   IF(CODE(22)-22.)57,53,57
 57   IF(CODE(20)-20.)58,53,58
 58   CALL GBZC (GB,ZC,AMCGB,GCGB,AMGB)
      CALL RPMHS (PC,TC,TB,HVB,EVB)
      GO TO 59
 53   CALL RPMHS (PC,TC,TB,HVB,EVB)
      CALL LZC (HVB,ZC)
 59   CALL GLVC (PC,TC,ZC,VC)
 47   IF(VB-0.)60,60,61
 61   GO TO 2222
 60   IF(CODE(10)-10.)62,63,62
 62   IF(CODE(18)-18.)64,63,64
   63 CALL  SVB (AVB,VB,GCS)
      GO TO 65
 64   CALL RENVB (VC,PC,VB)
 65   GO TO 2222
 2222 CONTINUE
C     END PART II
      RETURN
      END
```

```
      SUBROUTINE PO1 (PC,ZC,VC,VB,TB,TC,T,P,WT,NAME,FB,
     1CPO,ALPHA,W,Z1,Z2,Z3,VP,CP,CV,AA,V,Z,ZZ,*)
      DIMENSION NAME(20), FB(13)
      ZZ=0.
      PRINT 1040
  122 PRINT 1024,(NAME(NN),NN=1,7),T,P,WT
      IF(AA-0.)10,10,11
   11 PRINT 1070,Z1,Z2,Z3
      RETURN 1
   10 PRINT 1025,T
      PRINT 1026,P
      PRINT 1027,V
      PRINT 1028,Z
      PRINT 1029,TB
      PRINT 1030,VB
      PRINT 1031,TC
      PRINT 1032,PC
      PRINT 1033,VC
      PRINT 1034,ZC
      PRINT 1035,VP
      PRINT 1036,ALPHA
      PRINT 1037,W
      PRINT 1038,CPO
      IF(FB(1)-1.)143,144,143
  144 PRINT 1039
      ZZ=1.
  143 PRINT 1041,CP
      PRINT 1042,CV
 1024 FORMAT (1H0,36X,7A4/1H0,17X,'T=',F7.2,1X,'DEG K',
     15X,'P=',F7.2,1X,'ATM',5X,'MOLE WT=',F6.2/)
 1025 FORMAT (15X,F9.2,7X,'DEG K,',12X,'T'/)
 1026 FORMAT (15X,F9.2,7X,'ATM,',14X,'P'/)
 1027 FORMAT (15X,F9.2,7X,'CC/G MOLE,',8X,'V'/)
 1028 FORMAT (15X,F10.3,24X,'Z'/)
 1029 FORMAT (15X,F9.2,7X,'DEG K,',12X,
     1'NORMAL BOILING PT.'/)
 1030 FORMAT (15X,F9.2,7X,'CC/G MOLE,',8X,
     1'VOLUME AT NORMAL BOILING'/54X,'POINT'/)
 1031 FORMAT (15X,F9.2,7X,'DEG K,',12X,'TC'/)
 1032 FORMAT (15X,F9.2,7X,'ATM,',14X,'PC'/)
 1033 FORMAT (15X,F9.2,7X,'CC/G MOLE,',8X,'VC'/)
 1034 FORMAT (15X,F10.3,24X,'ZC'/)
 1035 FORMAT (15X,F10.3,6X,'ATM,',14X,'VAPOR PRESSURE'/)
 1036 FORMAT (15X,F9.2,25X,'RIEDEL FACTOR'/)
 1037 FORMAT (15X,F10.3,24X,'ACENTRIC FACTOR'/)
 1038 FORMAT (15X,F10.3,6X,'CAL/G MOLE-DEG K,',1X,'CPO'/)
 1039 FORMAT (1H+,61X,'*')
 1040 FORMAT (1H1,25X,'THE ESTIMATED PHYSICAL PROPERTIES'
     1,'OF')
 1041 FORMAT (15X,F10.3,6X,'CAL/G MOLE-DEG K,',1X,'CP'/)
```

```
 1042 FORMAT (15X,F10.3,6X,'CAL/G MOLE-DEG K,',1X,'CV'/)
 1070 FORMAT (15X,'Z FOUND TO BE TOO LARGE. THE  ROOTS',
     1'ARE',1X,3F5.1/)
      RETURN
      END
```

```
      SUBROUTINE PO2 (HVS,EVH,HF,EF,FET,ENGY,DIS,HSV,
     1DELH,DELS,FUGCOF,UG,DELTA,RHOR,U,THCU,THC,AA,
     2DIPOLE,BB,T,P,ZZ,HF298)
      DIMENSION BB(13)
      IF(BB(2)-2.)145,146,145
145   PRINT 1043,ENGY
      PRINT 1044,DIS
      PRINT 1045,HSV
      GO TO 147
 146  PRINT 1046,DIPOLE
      GO TO 145
147   IF(BB(3)-3.)150,149,150
 149  PRINT 1047,T
      GO TO 154
148   PRINT 1048,UG
      GO TO 157
150   IF(BB(4)-4.)152,151,152
151   PRINT 1049
      GO TO 154
 152  IF(BB(5)-5.) 148,153,148
153   PRINT 1050,DELTA
 154  IF(BB(6)-6.) 148,155,148
155   PRINT 1051,RHOR
156   IF(BB(7)-7.)157,158,157
158   PRINT 1052
      GO TO 169
157   IF(BB(8)-8.)159,160,159
160   PRINT 1053,RHOR
      GO TO 161
159   PRINT 1054,U
161   PRINT 1055,THCU
      IF(BB(9)-9.)165,164,165
163   PRINT 1056,THC
      GO TO 169
164   PRINT 1057,RHOR
      GO TO 169
165   IF(BB(10)-10.)167,166,167
166   PRINT 1058,P
      GO TO 169
167   IF(BB(11)-11.)163,168,163
168   PRINT 1059
169   PRINT 1060,DELH
      PRINT 1061,DELS
      PRINT 1062,FUGCOF
      PRINT 1063,EVH
      PRINT 1064,HVS
      IF(BB(13)-13.)170,171,170
171   PRINT 1065,HF298
      GO TO 174
170   IF(BB(12)-12.)172,173,172
```

```
 172  PRINT 1066,HF
      PRINT 1065,HF298
      GO TO 174
 173  PRINT 1067,T
      GO TO 176
 174  PRINT 1068,EF
      PRINT 1069,FFF
 176  IF(ZZ)20,20,175
 175  PRINT 1071
 20   PRINT 1072
 1043 FORMAT (15X,F9.2,7X,'DEG K,',12X,'E/K'/)
 1044 FORMAT (15X,F10.3,6X,'ANGSTROMS,',8X
     1,'INTERMOLECULAR DISTANCE'/)
 1045 FORMAT (15X,F9.2,7X,'CC/G MOLE,',8X,
     1'HARD-SPHERE VOLUME'/)
 1046 FORMAT (15X,F10.3,6X,'DEBYES,',11X,'DIPOLE MOMENT'/)
 1047 FORMAT (15X,'T TOO HIGH TO CALC. UO BY THEORETICAL',
     1' METHOD.  T=',F9.2/)
 1048 FORMAT (15X,F12.5,4X,'CENTIPOISE,',7X,'VISCOSITY ',
     1'AT LOW PRESSURE'/)
 1049 FORMAT (15X,'THEORETICAL METHOD NOT CONVERGING'/)
 1050 FORMAT (15X,'DELTA TOO HIGH TO CALC. UO BY THEOR',
     1'ETICAL METHOD'/20X,'DELTA=',F9.3/)
 1051 FORMAT (15X,'REDUCED DENSITY TOO HIGH TO CALC. ',
     1'UO BY STIEL AND THODOS'/20X,'METHOD.  RHOR=',F7.2/)
 1052 FORMAT (15X,'U CAN NOT BE CALC. DUE TO NO VALUE ',
     1'FOR UO.'/)
 1053 FORMAT (15X,'REDUCED DENSITY TOO HIGH TO CALC. U',
     1' BY JOSSI, STIEL, AND '/20X,'THODOS METHOD.  ',
     2'RHOR=',F7.2/)
 1054 FORMAT (15X,F12.5,4X,'CENTIPOISE,',7X,'VISCOSITY',
     1' AT ELEVATED'/54X,'PRESSURE'/)
 1055 FORMAT (15X,F14.7,2X,'CAL/CM-SEC-DEG K,',1X,'THER',
     1'MAL CONDUCTIVITY AT'/54X,'LOW PRESSURE'/1H1)
 1056 FORMAT (15X,F14.7,2X,'CAL/CM-SEC-DEG K,',1X,'THER',
     1'MAL CONDUCTIVITY AT'/54X,'ELEVATED PRESSURE'/)
 1057 FORMAT (15X,'REDUCED DENSITY TOO HIGH TO CALC. K.',
     1'  RHOR=',F7.2/)
 1058 FORMAT (15X,'P TOO HIGH TO CALC. K.  P=',F7.2/)
 1059 FORMAT (15X,'METHOD FOR K NOT APPLICABLE'/)
 1060 FORMAT (15X,F9.2,7X,'CAL/G MOLE,',7X,'H(IDEAL)-H',
     1'(IDEAL)-H(REAL)'/)
 1061 FORMAT (15X,F10.3,6X,'CAL/G MOLE-DEG K,',1X,'S(
     1,'IDEAL)-S(REAL)'/)
 1062 FORMAT (15X,F10.3,24X,'FUGACITY COEFFICIENT'/)
 1063 FORMAT (15X,F8.1,8X,'CAL/G MOLE,',7X,'HEAT OF '
     1,'VAPORIZATION'/54X,'AT NORMAL BOILING PT.'/)
 1064 FORMAT (15X,F10.3,6X,'CAL/G MOLE-DEG K,',1X,
     1'ENTROPY OF VAPORIZATION'/54X,'AT NORMAL BOILING'
     2,' PT.'/)
```

```
 1065 FORMAT (15X,F10.3,6X,'KCAL/G MOLE,',6X,'HEAT OF '
     1,'FORMATION FOR'/54X,'IDEAL GAS AT 1 ATM'/54X,
     2'AND 298 DEG K'/)
 1066 FORMAT (15X,F10.3,6X,'KCAL/G MOLE,',6X,'HEAT OF '
     1,'FORMATION AT'/54X,'STATED TEMPERATURE'/)
 1067 FORMAT (15X,'HEAT OF FORMATION AT T=',F7.2,1X,
     1'CAN NOT BE CALC. DUE TO'/20X,'STIPULATIONS ON '
     2,'METHODS.'/)
 1068 FORMAT (15X,F10.3,6X,'CAL/G MOLE-DEG K,',1X,'EN',
     1'TROPY OF FORMATION FOR'/54X,'IDEAL GAS AT 1 ATM'
     2/54X,'AND 298 DEG K.'/)
 1069 FORMAT (15X,F10.3,6X,'KCAL/G MOLE,',6X,'FREE EN',
     1'ERGY OF FORMATION'/54X,'FOR IDEAL GAS AT 1'/54X,
     2'ATM AND 298 DEG K.'/)
 1071 FORMAT (1H0,14X,'CPJ WAS CALC. BY X 2 EVEN THOUGH'
     1,' METHOD WAS NOT APPLICABLE.')
 1072 FORMAT (1H0)
      RETURN
      END
```

```
      SUBROUTINE TRACA (P,AAC,BAC,CAC,TBAC)
C     BOILING POINT AT PRESSURE P VIA ANTOINE-COX EQN.
      TBAC=-BAC/(ALOG10(P)-AAC)+CAC
      RETURN
      END
```

```
      SUBROUTINE P04 (DENS,DELH,HTCAP,VISC,VCSND,WT,
     1APARC,DELTA,SORTE,CONTL,T,P,PC,TC,VC,
     2ATRH,ATRL,APRH,APRL,SATL)
      DR=(DENS*1000.0/WT)*VC
      PRINT 15
      TR=T/TC
      IF(TR-1.0) 101,50,50
   50 PRINT 14
      GO TO 51
  101 PRINT 2,DENS
      IF(SATL-1.0) 70,70,71
   70 PRINT 16
      GO TO 72
   71 PRINT 17
   72 IF(APRH) 90,90,91
   91 PRINT 19
      GO TO 150
   90 IF(APRL) 92,92,93
   93 PRINT 20
      GO TO 150
   92 CONTINUE
      IF(ATRH) 80,80,81
   81 PRINT 18
      GO TO 150
   80 IF(ATRL) 82,82,83
   83 PRINT 21
      GO TO 150
   82 CONTINUE
  102 PRINT 3,DELH
  150 CONTINUE
      IF(DR-2.0) 305,306,306
  305 PRINT 23
  306 IF(TR-.6) 300,301,301
  300 PRINT 22
  301 CONTINUE
  103 PRINT 4,HTCAP
      IF(VISC) 910,911,911
  910 PRINT 40
      GO TO 106
  911 CONTINUE
  104 PRINT 5,VISC
  106 PRINT 7,APARC
      IF(DELTA) 108,200,108
  200 PRINT 24
      GO TO 109
  108 PRINT 9,DELTA
  109 PRINT 10,SORTE
  110 PRINT 11,CONTL
   51 CONTINUE
    2 FORMAT (15X,F10.4,6X,'GRAMS/CC',9X,'LIQUID DENSITY'/)
```

```
    3 FORMAT (15X,F10.4,6X,'CAL/G MOLE',7X,'LIQ. ENTHALPY',
     11X,'DEPARTURE'/)
    4 FORMAT (15X,F10.4,6X,'CAL/G MOLE-C',5X,'HT CAPACITY',
     11X,'DEPARTURE'/)
    5 FORMAT (15X,F10.4,6X,'CENTIPOISE',7X,'LIQ VISCOSITY'/)
    7 FORMAT (15X,F10.4,6X,'(DYNES/CM)**1/4(CC/G MOLE)',2X,
     1'PARACHOR'/)
    9 FORMAT (15X,F10.4,6X,'CAL/G MOLE-K',5X,'LIQ ENTROPY',
     11X,'DEPARTURE'/)
   10 FORMAT (15X,F10.6,6X,'DYNES/CM',9X,'SURFACE TENSION'/)
   11 FORMAT (15X,F10.6,6X,'1/DEG K',10X,'COEFF OF THRMAL EXP'/)
   13 FORMAT (15X,F10.4,5X,'CAL/G MOLE',7X,'LATENT HT OF',
     1'VAPORIZATION AT'/,14X,14X,14X,12X,F6.2,2X,'ATM'/)
   14 FORMAT (15X,'REDUCED TEMP>1.0,',
     1' DENSITY NOT CALCULATED',/,15X,'PROGRAM DUMPED')
   15 FORMAT (1H1,15X,'LIQUID PHYSICAL PROPERTIES'/,/)
   16 FORMAT (15X,'SATURATED LIQUID ENTHALPY CALC')
   17 FORMAT (15X,'COMPRESSED LIQUID ENTHALPY CALC')
   18 FORMAT (15X,'METHOD NOT VALID-TR>1.0')
   19 FORMAT (15X,'METHOD NOT VALID-PR>1.0')
   20 FORMAT (15X,'METHOD NOT VALID-PR<1.0')
   21 FORMAT (15X,'METHOD NOT VALID-TR<0.5')
   22 FORMAT (15X,'REDUCED TEMPERATURE<0.6 FOR BWR METHOD')
   23 FORMAT (15X,'REDUCED DENSITY>2.0 FOR BWR METHOD')
   24 FORMAT (15X,'ISOTHERMAL ENTROPY DEPARTURE CANNOT'/,
     115X,'BE CALCULATED'/)
   40 FORMAT (15X,'VISCOSITY CANNOT BE CALCULATED-NO INPUT DATA')
      RETURN
      END
```

```
  786          SUBROUTINE COTE(TC,COFTE,T)
  787 C        COEFFICIENT OF THERMAL EXPANSION
  788          COFTE=.04214/(TC-T)**0.641
  789          RETURN
  790          END
```

```
      SUBROUTINE YWDEN(ZC,TC,T,VC,P,PC,DENS,DELPR,WT)
C     LIQUID DENSITY VIA YEN WOODS CORRELATION
      PR=P/PC
      TR=T/TC
      AA=17.4425-214.578*ZC+989.625*ZC*ZC-1522.06*ZC*ZC*ZC
      IF(ZC-.26) 111,111,110
  110 BB=60.2091-402.063*ZC+501.0*ZC*ZC+641.0*ZC*ZC*ZC
      GO TO 120
  111 BB=-3.28257+13.6377*ZC+107.4844*ZC*ZC-384.211*ZC*ZC*ZC
  120 D=0.93-BB
      RRS=1.0+AA*(1.-TR)**.3333+BB*(1.0-TR)**.6667+D*(1.0-TR)
     1**1.3333
      DENS=RRS/VC*WT
      AAF=245.2568*ZC-871.2178*ZC**3.+(0.1059795/ZC**3.)-53.36101
      DELPR=PR-EXP(2.303*AAF*(1.0-1.0/TR))
      IF(DELPR) 150,150,210
  150 GO TO 500
  210 IF(ZC-.27) 130,135,140
  135 DELT=0.0
      GO TO 311
  130 IF(ZC-.25) 131,132,132
  131 A1=.049
      A2=-.4344
      A3=.7915
      A4=-.7654
      A5=.3367
      B1=.0674
      B2=-.06109
      B3=.00201
      B4=-.2371
      B5=.1602
      C1=-.01393
      C2=-.003459
      C3=-.1611
      C4=0.0
      D1=-6.55
      D2=7.4027
      D3=15.344
      D4=-37.04
      D5=20.169
      GO TO 136
  132 A1=.093
      A2=-.3445
      A3=.4042
      A4=-.2065
      A5=.05475
      B1=.022
      B2=-.003564
      B3=-.07960
      B4=.06546
```

```
      B5=-.0217
      C1=.01737
      C2=-.03035
      C3=.06310
      C4=0.0
      D1=-16.0
      D2=30.090
      D3=19.645
      D4=-61.305
      D5=47.031
      GO TO 136
  140 A1=-.0817
      A2=.3274
      A3=-.5014
      A4=.567
      A5=-.1341
      B1=-.023
      B2=-.0124
      B3=.1625
      B4=-.2155
      B5=.08643
      C1=.05525
      C2=-.3518
      C3=.5194
      C4=-.3509
      D1=-21.0
      D2=55.175
      D3=-33.637
      D4=-28.109
      D5=25.277
  136 EYF=A1+A2*(1.0-TR)**.3333+A3*(1.0-TR)**.6667+A4*(1.0-TR)**1.0+
     1A5*(1.0-TR)**1.333
      XJ=B1+B2*(1.0-TR)**.3333+B3*(1.-TR)**.6667+B4*(1.0-TR)+B5*
     1(1.0-TR)**1.3333
      XK=C1+C2*TR+C3*TR*TR+C4*TR*TR*TR
      XL=D1+D2*(1.-TR)**.3333+D3*(1.-TR)**.6667+D4*(1.0-TR)+D5*
     1(1.-TR)**1.3333
      IF(DELPR-.2) 310,137,137
  137 DELT=EYF+XJ*ALOG(DELPR)+XK*EXP(XL*DELPR)
      GO TO 311
  310 DELT1=EYF+XJ*(-1.60944)+XK*EXP(XL*.2)
      DELT=DELT1*DELPR/.2
  311 EE=.714-1.620*(1.-TR)**.3333-.646*(1.-TR)**.6667+3.690*(1.-TR)
     1-2.190*(1.-TR)**1.3333
      FF=.2[illegible]TR**2.0907/(1.+.6*(-ALOG(TR))**.641)
      GG=.05+5.221*(1.01-TR)**.75*EXP(-7.348*(1.01-TR))
      HH=-10.0+45.22*(1.-TR)**.3333-103.79*(1.-TR)**.6667+114.44
     1*(1.-TR)-47.34*(1.-TR)**1.3333
      IF(DELPR-.2) 312,313,313
  312 DELH=(EE+FF*(-1.60944)+GG*EXP(HH*.2))*DELPR/.2
```

```
 301        GO TO 315
 302   310  DELT=EE+FF*ALOG(DELPR)+GG*EXP(HH*DELPR)
 303   315  TR=(.5+DELP)*DELT
 304        DENS=WR/VC*WT
 305   500  CONTINUE
 306        RETURN
 307        END
```

```
       SUBROUTINE SPARC(ANCG,ANCGC,APARC,BONDS)
C      PARACHOR VIA MCGOWAN ADDITIVE METHOD
       DIMENSION ANCG(9),ANCGC(9)
       SUMPA=0.0
       DO 190 N=1,9
   190 SUMPA=ANCG(N)*ANCGC(N)+SUMPA
       APARC=SUMPA-19.0*BONDS
       RETURN
       END
```

```
    907          SUBROUTINE SURT (APARC,DENS,WT,TB,SURTE,T,TC,
    908         1SURTT,TTTT)
    909          SURFACE TENSION VIA PARACHOR METHOD
    910          IF(SURTT) 1,2,1
    911        1 TR=T/TC
    912          SURTE=SURTT*((1.0-TR)/(1.0-TTTT/TC))**1.22
    913          RETURN
    914          CONTINUE
    915          DENVB=WT/(82.06*TB)
    916          DENV=DENVB*10.**(5.0*(T/TB-1.0))
    917          SURTE=(APARC*(DENS-DENV)/WT)**4.0
    918          RETURN
    919          END
```

```
      SUBROUTINE BWRCP(T,DENS,A,B,C,A0,B0,C0,HTCAP,ALPH,GAMM,
     1APP,BPP,CPP,A0PP,B0PP,C0PP,ALPP,GAMPP,R,TC,PC,W,DDDD,WT)
C     LIQUID HEAT CAPACITY VIA BWR EQUATION OF STATE
      DIMENSION APP(4),A0PP(4),BPP(4),B0PP(4),CPP(4),C0PP(4),
     1ALPP(4),GAMPP(4)
      DENS=DENS*1000.0/WT
      IF(DDDD-1.0) 2,1,2
    2 K=3.0
      GO TO 3
    1 K=1.0
    3 R=.08205
      AP=APP(K)+APP(K+1)*W
      A0P=A0PP(K)+A0PP(K+1)*W
      BP=BPP(K)+BPP(K+1)*W
      B0P=B0PP(K)+B0PP(K+1)*W
      CP=CPP(K)+CPP(K+1)*W
      C0P=C0PP(K)+C0PP(K+1)*W
      ALPHP=ALPP(K)+ALPP(K+1)*W
      ALPHP=ALPHP/AP
      GAMMP=GAMPP(K)+GAMPP(K+1)*W
      F1=TC*TC*R*R/PC
      A=AP*F1*TC*R/PC
      A0=A0P*F1
      B=BP*F1/PC
      B0=B0P*R*TC/PC
      C=CP*F1*F1*TC/R
      C0=C0P*F1*TC*TC
      ALPH=ALPHP*F1*TC*R/(PC*PC)
      GAMM=GAMMP*F1/PC
      D2=DENS*DENS
      T2=T*T
      T3=T2*T
      D5=D2*D2*DENS
      DEX=EXP(-GAMM*D2)
      Z1=R+B0*R*DENS+2.0*C0*DENS/T3+B*R*D2-2.*C*D2*(1.+GAMM*D2)
     1*DEX/T3
      Z2=R*T+2.*DENS*(B0*R*T-A0-C0/T2)+3.*D2*(B*R*T-A)+
     16.0*A*ALPH*D5+C*D2*DEX*(3.+3.*GAMM*D2+2.0*GAMM*GAMM
     2*D2*D2)/T2
      Z3=6.0*C0*DENS/T3
      Z4=6.0*C*(DEX-1.0)/(T3*GAMM)+3.0*C*D2*DEX/T3
      HTCAP=T*Z1*Z1/Z2+Z3+Z4-R
      DENS=DENS*WT/1000.0
      RETURN
      END
```

```
          SUBROUTINE ENTYA (T,P,DENS,PC,TC,VC,ZC,WT,DELH,DELPR,
         1ATRH,ATRL,APRH,APRL,SATL)
C         ISOTHERMAL ENTHALPY DEVIATION VIA YEN AND ALEXANDER
          SATL=0.0
          APRL=0.0
          APRH=0.0
          ATRH=0.0
          ATRL=0.0
          IF(ZC-0.24) 200,200,205
  200     NZ=1
          GO TO 240
  205     IF(ZC-0.26) 210,210,215
  210     NZ=2
          GO TO 240
  215     IF(ZC-.28) 220,220,230
  220     NZ=3
          GO TO 240
  230     NZ=4
  240     CONTINUE
          PR=P/PC
          IF(PR-1.0) 1,2,2
    1     IF(PR-.01) 3,5,5
    2     APRH=1.0
          GO TO 5
    3     APRL=1.0
    5     CONTINUE
          IF(DELPR) 305,305,370
  305     PR=P/PC
          TR=T/TC
          SATL=1.0
          GO TO (330,335,340,345),NZ
  330     DELH=-TC*(7.+4.3667*(-ALOG(PR))**.333)/(1.+.004*ALOG(PR))
          GO TO 350
  335     DELH=-TC*(6.5+4.4*(-ALOG(PR))**0.3952)/(1.0-0.00165*ALOG(PR))
          GO TO 350
  340     DELH=-TC*(5.8+5.19*(-ALOG(PR))**.4965)/(1.-.1*ALOG(PR))
          GO TO 350
  345     DELH=-TC*(5.4+3.6465*(-ALOG(PR)))/(1.-0.0036942*ALOG(PR))
  350     CONTINUE
          DELH=DELH/1.8
  360     CONTINUE
  370     CONTINUE
          PR=P/PC
          TR=T/TC
          IF(DELPR) 555,655,559
  559     CONTINUE
          SATL=2.0
          IF(TR-1.0) 6,7,7
    6     IF(TR-0.5) 8,9,9
    7     ATRH=1.0
```

```
          GO TO 9
        8 ATHL=1.0
        9 CONTINUE
          GO TO (605,610,615,620),K7
      605 CONTINUE
          DELH=-TC*(-.086443*(PR-4.2)-12.93879*(TR-.77)+10.41311*(TR-.
         177)**2-.1568094*(PR-4.2)*(TR-.77)+.7466342*ALOG(PR)+3.17422*
         2ALOG(PR)*ALOG(TR)+2.930566*ALOG(PR)*(ALOG(TR))**2+12.724291)
          GO TO 625
      610 CONTINUE
          DELH=-TC*(-.1074635*(PR-4.2)-15.60132*(TR-.77)-15.18611*(TR-.7
         17)**2-.1476876*(PR-4.2)*(TR-.77)+.7600774*ALOG(PR)+5.15466*ALO
         2G(PR)*ALOG(TR)+2.366538*ALOG(PR)*ALOG(TR)*ALOG(TR)+12.28618)
          GO TO 625
      615 CONTINUE
          DELH=-TC*(-.1363774*(PR-4.064)-14.56975*(TR-.79749)-7.612724*(
         1TR-.79749)**2-.1642468*(TR-.79749)*(PR-4.064)+1.636605*ALOG(PR)+
         24.463472*ALOG(PR)*ALOG(TR)+4.525831*ALOG(PR)*(ALOG(TR))**2
         3+10.06085)
          GO TO 625
      620 CONTINUE
          DELH=-TC*(-.0957211*(PR-4.2)-9.501235*(TR-.77)-17.30389*(TR-.
         177)**2-.5195707*(PR-4.2)*(TR-.77)+1.566092*ALOG(PR)+4.2271*AL
         2OG(PR)*ALOG(TR)+3.13164*ALOG(PR)*ALOG(TR)*ALOG(TR)+9.707447)
      625 CONTINUE
          DELH=DELH/1.8
      650 CONTINUE
      655 CONTINUE
          RETURN
          END
```

```
 1045           SUBROUTINE EVIS (GASS,TC,TTT,VISCPT,T,ZC,VC,P,PC,WT,
 1046          1VISC)
 1047 C         LIQUID VISCOSITY VIA THOMAS METHOD
 1048           IF(VISCPT) 817,815,817
 1049      817  CONTINUE
 1050           PR=1.0/PC
 1051           TR=TTT/TC
 1052           AA=17.4425-214.578*ZC+989.625*ZC*ZC-1522.06*ZC*ZC*ZC
 1053           IF(ZC-.26) 111,111,110
 1054      110  BB=60.2091-402.063*ZC+501.0*ZC*ZC+641.0*ZC*ZC*ZC
 1055           GO TO 120
 1056      111  BB=-3.28257+13.6377*ZC+107.4844*ZC*ZC-384.21*ZC*ZC*ZC
 1057      120  D=0.93-BB
 1058           VPS=1.0+AA*(1.-TR)**.3333+BB*(1.0-TR)**.6667+D*(1.0-TR)
 1059          1**1.3333
 1060           DENSI=RRS/VC*WT
 1061           AAH=245.2568*ZC-571.2178*ZC**3.+(0.1039735/ZC**3.)-33.5616
 1062           DELPR=PR-EXP(2.303*AAH*(1.0-1.0/TR))
 1063           IF(DELPR) 150,150,210
 1064      150  GO TO 500
 1065      210  IF(ZC-.27) 130,135,140
 1066      135  DELT=0.0
 1067           GO TO 311
 1068      130  IF(ZC-.25) 131,132,132
 1069      131  A1=.069
 1070           A2=-.4344
 1071           A3=.7915
 1072           A4=-.7654
 1073           A5=.5567
 1074           B1=.0674
 1075           B2=-.06109
 1076           B3=.00251
 1077           B4=-.2378
 1078           B5=.1605
 1079           C1=-.01393
 1080           C2=-.003459
 1081           C3=-.1511
 1082           C4=0.0
 1083           D1=-3.35
 1084           D2=7.3027
 1085           D3=-13.344
 1086           D4=-37.04
 1087           D5=20.169
 1088           GO TO 136
 1089      132  A1=.078
 1090           A2=-.3445
 1091           A3=.0442
 1092           A4=-.2383
 1093           B1=.05473
 1094            1=.022
```

```
      B2=-.00565
      B3=-.07760
      B4=.05045
      B5=-.0217
      C1=.01937
      C2=-.03055
      C3=.06310
      C4=0.0
      D1=-16.0
      D2=30.099
      D3=17.045
      D4=-31.305
      D5=47.031
      GO TO 136
  140 A1=-.0617
      A2=.0274
      A3=-.0014
      A4=.037
      A5=-.1342
      B1=-.023
      B2=-.0124
      B3=.1625
      B4=-.2135
      B5=.08543
      C1=.00026
      C2=-.3516
      C3=.0194
      C4=-.3809
      D1=-21.0
      D2=55.174
      D3=-53.667
      D4=-24.109
      D5=23.277
  136 FYE=A1+A2*(1.0-TR)**.3333+A3*(1.0-TR)**.6667+A4*(1.0-TR)**1.0+
     1A5*(1.0-TR)**1.333
      XU=B1+B2*(1.0-TR)**.3333+B3*(1.-TR)**.6667+B4*(1.0-TR)+B5*
     1(1.0-TR)**1.3333
      XK=C1+C2*TR+C3*TR*TR+C4*TR*TR*TR
      XL=D1+D2*(1.-TR)**.3333+D3*(1.-TR)**.6667+D4*(1.0-TR)+D5*
     1(1.-TR)**1.3333
      IF(DELPR-.2) 310,137,137
  137 DELT=FYE+XU*ALOG(DELPR)+XK*EXP(XL*DELPR)
      GO TO 311
  310 DELT1=FYE+XU*(-1.60944)+XK*EXP(XL*.2)
      DELT=DELT1*DELPR/.2
  311 ZF=.734-1.626*(1.-TR)**.3333-.640*(1.-TR)**.6667+5.699*(1.-TR)
     1-2.306*(1.-TR)**1.3333
      PF=.786*TR**2.0427/(1.+EXP(-ALOG(TR))**.44))
      WS=.35+.221*(1.01-TR)**.75*EXP(-7.24*(1.01-TR))
      WR=-10.0+45.22*(1.-TR)**.3333-103.79*(1.-TR)**.6667+114.44
```

```
 1145          F=(1.0-TK)-47.5*([illegible])**[illegible]
 1146          IF(TTLK-.2) [illegible]
 1147    312   DELT=(F0+F1*(-1.0[illegible])-G0*EXP(HM*.2))*DELPR/.2
 1148          GO TO 315
 1149    311   DELT=[illegible]*ALOG(DELPR)+G0*EXP(HM*DELPR)
 1150    315   [illegible]DELPR*DELT
 1151          DENS=RK/VC*T
 1152    500   CONTINUE
 1153          TR=TTT/TC
 1154          TK=T/TC
 1155          TAK=ALOG10(3.569*VISCPT/(DENS**0.5))/(1.0/TR-1.0)
 1156          VISC=((DENS**0.5)/3.569)*10.0**(TAK*(1.0/TR-1.0))
 1157          RETURN
 1158    31    VISC=-1.0
 1159          RETURN
 1160          END
```

```
      SUBROUTINE BENEDT (P,PC,T,TC,VC,BENTA,
     1DELGB1,GENS,ALPHA,ZC)
C     ISOTHERMAL EFF BY DEPARTURE VIA HIRSCHFELDER,
C     BUEHLER,MCGEE,AND SUTTON EQUATION OF STATE
      DIMENSION A(4,6),AWC(4),AMC(4),AG(4),AW(4),
     1AT(4)
      B=1.0
      BETA=4.0
      X=0.352
      Y=ABS(ZC-X)
      IF(Y-.001) 50,50,51
   59 B=B/10.0
   51 IF(ZC-X) 52,50,54
   55 IF(ZC-X) 52,50,54
   52 BETA=BETA+B
      X=BETA*(3.0*BETA-1.0)/(1.0+BETA)**3.0
      Y=ABS(ZC-X)
      IF(Y-.001) 50,50,55
   54 B=B*10.0
   57 B=B/100.0
   56 BETA=BETA-B
      X=BETA*(3.0*BETA-1.0)/(1.0+BETA)**3.0
      Y=ABS(ZC-X)
      IF(Y-.001) 50,50,58
   58 IF(ZC-X) 59,50,56
   50 CONTINUE
      AKO=5.5
      AK1=BETA-AKO
      AK2=(1.0-AKO-ALPHA+2.0*BETA)/3.0
      B=(1.0/BETA)*(3.0*BETA*BETA-5.0*BETA-1.0)
     1/(3.0*BETA-1.0)
      C1=(BETA-3.0)/(3.0*BETA-1.0)
      AK3=B/(4.0*C1-B*B)**0.5
      AK4=2.0*C1/(4.0*C1-B*B)**0.5
      DR=[illegible]*VC/[illegible]
      TR=T/TC
      V1=2.0*DR*(AKO/TR+AK1/(TR*TR))
      V2=1.5*AK2*DR*DR*(1.0-1.0/(TR*TR))
      V3=ALOG(DR*TR)+([illegible]*DR)/(1.0-B*DR-C1*DR*DR)
     1-0.5*ALOG(1.0-B*DR-C1*DR*DR)
      V4=AK3*ATAN(AK3)+AK3*ATAN(AK4*DR-AK3)-ALOG(ZC)
      GT=-ZC*V1-ZC*V2+V3+V4
      A(1,1)=0.0
      A(1,2)=0.0
      A(1,3)=0.0
      A(1,4)=0.5-BETA
      A(1,5)=-2.25-ALPHA/2.0+BETA
      A(1,6)=0.0
      A(2,1)=[illegible].5-3.18*BETA
      A(1,2)=-313.5+13.4*BETA
```

```
      A(2,3)=400.0-71.3*BETA
      A(2,4)=-237.4+15.4*BETA
      A(2,5)=47.0-4.06*BETA
      A(2,6)=0.0
      A(3,1)=-124.4+65.19*BETA+0.303*BETA*BETA
      A(3,2)=429.0-7.64*BETA-1.815*BETA*BETA
      A(3,3)=-520.0+1.94*BETA+3.05*BETA*BETA
      A(3,4)=253.0+15.7*BETA-3.65*BETA*BETA
      A(3,5)=ALPHA/2.0-27.05-10.09*BETA+1.015*BETA*BETA
      A(3,6)=-5.44+4.00*BETA-0.303*BETA*BETA
      A(4,1)=44.4-5.22*BETA
      A(4,2)=-156.9+16.92*BETA
      A(4,3)=204.5-25.44*BETA
      A(4,4)=-115.5+15.0*BETA
      A(4,5)=25.7-3.26*BETA
      A(4,6)=0.0
      DR=PC*S*VC/WT
      DR2=DR*DR
      DR4=DR2*DR2
      DO 2 J=1,4
      ABC(J)=(A(J,1)+A(J,2)*DR+A(J,3)*DR2+A(J,4)*DR2*DR
     1+A(J,5)*DR4+A(J,6)*DR4*DR)/DR
    2 AAC(J)=(-0.5*A(J,1)-A(J,2)*DR+A(J,3)*DR2*ALOG(DR)
     1+A(J,4)*DR2*DR+0.5*A(J,5)*DR4+A(J,6)*DR4*DR/3.0)
     2/DR2
      R=82.056
      PI=3.1415927
      Y=0.4278*R*R*TC**2.5/PC
      B=0.0867*R*TC/PC
      QQ=P*Y/(R*R*T**2.5)-P*P*B*B/(R*R*T*T)-B*P/(R*T)
      RR=-P*P*Y*B/(R*R*R*T**3.5)
      C=1.0/3.0
      ALPHA=QQ-C
      BETA=RR+QQ/3.0-2.0/27.0
      TAU=BETA*BETA/4.0+ALPHA*ALPHA*ALPHA/27.0
      IF(TAU) 10,11,12
C     ONE REAL ROOT
   12 Z=((-BETA/2.0+SQRT(TAU))**C)+((-BETA/2.-SQRT(TAU))
     1**C)+C
      GO TO 99
C     THREE REAL ROOTS, AT LEAST TWO OF WHICH ARE EQUAL
   11 Z1=-2.*((-BETA/2.)**C)+C
      Z2=((-BETA/2.)**C)+C
      IF(Z1) 20,20,30
   20 IF(Z2-0.0) 31,31,33
   31 Z=Z2
      GO TO 99
   30 IF(Z1-0.0) 32,32,20
   32 Z=Z1
      GO TO 99
```

```
   50 Z3=0.0
      GO TO 22
C     THREE REAL AND UNEQUAL ROOTS
   10 OMEGA=SQRT(((BETA*BETA)/4.)/((-ALPHA**3)/27.))
      THETA=ATAN(SQRT((1./OMEGA)*(1./OMEGA)-1.))
      IF(BETA) 13,14,14
   13 THETA=PI-THETA
   14 IF(BETA) 15,15,16
   15 F=2.0
      GO TO 17
   16 F=-2.0
   17 Z1=F*SQRT(-ALPHA/3.)*COS(THETA/3.)-C
      Z2=F*SQRT(-ALPHA/3.)*COS(THETA/3.+PI/3.)-C
      Z3=F*SQRT(-ALPHA/3.)*COS(THETA/3.+2.*PI/3.)-C
      IF(Z1) 18,18,19
   19 IF(Z1-5.) 25,18,18
   18 IF(Z2) 21,21,20
   20 IF(Z2-5.) 26,21,21
   21 IF(Z3) 22,22,24
   24 IF(Z3-5.) 27,22,22
   22 GO TO 987
   25 Z=Z1
      GO TO 99
   26 Z=Z2
      GO TO 99
   27 Z=Z3
   99 CONTINUE
      V=Z*R*T/P
      GO TO 995
  987 DELTA=0.0
      GO TO 500
  995 DR=VC/V
      DR2=DR*DR
      DR4=DR2*DR2
      DO 3 J=1,4
      AJ(J)=(A(J,1)+A(J,2)*DR+A(J,3)*DR2+A(J,4)*DR2*DR
     1+A(J,5)*DR4+A(J,6)*DR4*DR)/DR
    3 AT(J)=(-0.5*A(J,1)-A(J,2)*DR+A(J,3)*DR2*ALOG(DR)
     1+A(J,4)*DR2*DR+0.5*A(J,5)*DR4+A(J,6)*DR4*DR/3.0)
     2/DR2
      SUMF=0.0
      AT(1)=1.0/(TR*TR)
      AT(2)=1.0/TR
      AT(3)=1.0
      AT(4)=TR
      DO 1 J=1,4
    1 SUMF=AT(J)*(AJ(J)/DR-AGC(J)/(DENS*VC/RT)*AR(J)
     1-AGC(J))
      FUG=Z*SUMF+AZ
      P=0.0205
```

```
1311          OFFIAN=DLLN/I-KSPAN
1312     500  CONTINUE
1313          RETURN
1314          END
```

```
  1315        SUBROUTINE LYDTC (TB,THETA,TC)
  1316 C      TC BY LYDERSEN'S METHOD (T 1)
  1317        TC=TB/THETA
  1318        RETURN
  1319        END
```

```
      SUBROUTINE LYDTC (TCLYD,THETA,GCLYD)
C     FORMULA BY LYDERSEN'S METHOD (I 1)
      DIMENSION TCLYD(41),GCLYD(41)
      X=0.0
      SUMTC=0.0
      DO 15 I=1,41
   15 SUMTC=SUMTC+TCLYD(I)*GCLYD(I)
      X=GCLYD(25)*.021+X
      X=GCLYD(31)*.032+X
      X=GCLYD(14)*.062+X
      X=GCLYD(32)*.020+X
      X=GCLYD(33)*.012+X
      X=GCLYD(34)*.000+X
      X=GCLYD(35)*.000+X
      X=GCLYD(36)*.019+X
      X=GCLYD(37)*.000+X
      X=GCLYD(38)*.040+X
      X=GCLYD(39)*.031+X
      X=GCLYD(40)*.014+X
      X=GCLYD(41)*.015+X
      SUMTC=SUMTC-X
      THETA=0.567+SUMTC-SUMTC*SUMTC
      RETURN
      END
```

```
 1344          SUBROUTINE LYOPC (PCLY,T,PC,OCLYD)
 1345 C        C CALC LYO[illegible] (1/ 1)
 1346          DIMENSION PCLYD(41),OCLYD(41)
 1347          X=0.0
 1348          SUMP=0.0
 1349          DO 11 N=1,41
 1350       11 SUMP=SUMP+PCLYD(N)*OCLYD(N)
 1351          X=OCLYD(25)*.160+X
 1352          X=OCLYD(31)*.060+X
 1353          X=OCLYD(14)*.00+X
 1354          X=OCLYD(32)*.227+X
 1355          X=OCLYD(33)*.210+X
 1356          X=OCLYD(34)*.210+X
 1357          X=OCLYD(35)*.190+X
 1358          X=OCLYD(36)*.194+X
 1359          X=OCLYD(37)*.194+X
 1360          X=OCLYD(38)*.290+X
 1361          X=OCLYD(39)*.135+X
 1362          X=OCLYD(40)*.170+X
 1363          X=OCLYD(41)*.270+X
 1364          SUMP=SUMP-X
 1365          PC=T/(.34+SUMP)**2.
 1366          RETURN
 1367          END
```

```
 1368          SUBROUTINE GAZC (GB,ZC,ANCHB,GCGP,ANGB)
 1369 C        ZC VIA ADDITIVE TECHNIQUE (GARCIA-BARCENA)
 1370          DIMENSION GB(55),GCGP(10),ANGB(10)
 1371          SUMZ=0.0
 1372          I=0
 1373    11    I=I+1
 1374          IF(GCGP(I)-31.)12,13,15
 1375    12    IF(GCGP(I)-30.)16,17,16
 1376    17    SUMZ=SUMZ-(0.0360+0.0040*ANCHB)*ANGB(I)
 1377          GO TO 11
 1378    16    IF(GCGP(I)-32.)18,17,18
 1379    18    J=GCGP(I)
 1380          SUMZ=SUMZ-(GB(J))*ANGB(I)
 1381          GO TO 11
 1382    13    ZC=0.2905+SUMZ
 1383    15    CONTINUE
 1384          RETURN
 1385          END
```

```
 1386           SUBROUTINE GLZC (PC,TC,VC,ZC)
 1387 C         ZC BY USE OF GAS LAW (EQN 2)
 1388           R=82.056
 1389           ZC=PC*VC/(R*TC)
 1390    12     CONTINUE
 1391           RETURN
 1392           END
```

```
 1393          SUBROUTINE LZC (HV ,ZC)
 1394 C        ZC BY LYDERSEN'S METHOD (III 3)
 1395          ZC=1./(3.45+0.0000000067*HV*HV)
 1396    11    CONTINUE
 1397.         RETURN
 1398          END
```

```
1399          SUBROUTINE LYDVC (VCLYD,VC,GCLYD)
1400 C        VC VIA LYDERSEN METHOD  (IV 1)
1401          DIMENSION VCLYD(41),GCLYD(41)
1402          X=0.0
1403          SUMV=0.0
1404          DO 11 N=1,41
1405       11 SUMV=SUMV+VCLYD(N)*GCLYD(N)
1406          X=GCLYD(25)*25.0+X
1407          X=GCLYD(31)*14.0+X
1408          X=GCLYD(14)*11.0+X
1409          X=GCLYD(52)*55.0+X
1410          X=GCLYD(53)*51.0+X
1411          X=GCLYD(54)*41.0+X
1412          X=GCLYD(55)*36.0+X
1413          X=GCLYD(56)*45.0+X
1414          X=GCLYD(57)*35.0+X
1415          X=GCLYD(58)*60.0+X
1416          X=GCLYD(39)*57.0+X
1417          X=GCLYD(40)*42.0+X
1418          X=GCLYD(41)*53.0+X
1419          VC=SUMV-X+40.0
1420          RETURN
1421          END
```

```
 1422           SUBROUTINE GLVC (PC,TC,ZC,VC)
 1423  C        VC BY USE OF GAS LAW (IV 2)
 1424           R=82.056
 1425           VC=ZC*TC*R/PC
 1426    12     CONTINUE
 1427           RETURN
 1428           END
```

```
      SUBROUTINE [illegible] (TC,PC,TR,ALPHA,W)
C     ... Y EQN OF DEFINITION (V 1) .
      TR=0.7
      A3=36./TR+42.*ALOG10(TR)-35.-TR**6
      A2=0.0395*A3-ALOG10(TR)
      A1=0.3113*A3-7.*ALOG10(TR)
      PVPR=-A1-(ALPHA-7.)*A2
      VPR=10.**PVPR
      VP=VPR*PC
      IF(VP-1.075)5,5,6
    6 TBR=TB/TC
      H=TBR*(ALOG10(PC)/(1.-TBR))
      G=0.2271+0.4525*H
      D=(H/G-(1.+TBR))/((3.+TBR)*(1.-TBR))
      PVPR=-(G/TR)*(1.-TR*TR+D*(1.-TR)**3)
    5 W=-PVPR-1.0
   11 CONTINUE
      RETURN
      END
```

```
        SUBROUTINE SP[illegible] ([illegible])
C       [illegible] REGISTER [illegible] (V 2)
        J=([illegible]./7.)*(THETA/(1.-THETA))*ALOG10(PC)-1.
   12   CONTINUE
        RETURN
        END
```

```
1454          SUBROUTINE ALPHA (TB,TC,PC,ALPHA)
1455 C        RIEDEL FACTOR BY RIEDEL METHOD (VI 1)
1456          TR=TB/TC
1457          A=36./TR+42.*ALOG(TR)-35.-TR**6
1458          PSI=0.0364*A-ALOG10(TR)
1459          PHI=0.118*A-7.0*ALOG10(TR)
1460          ALPHA=(ALOG10(PC)-PHI)/PSI+7.00
1461    12    CONTINUE
1462          RETURN
1463          END
```

```
[illegible] RELEASE [illegible]     ALPHA     SUBROUTINE                  83/12/7[illegible]     PAGE

1444                   [illegible] ALPHA (J,ALPHA)
1445 C       INTEGRAL FACTOR BY [illegible] METHOD (VI 2)
1446         ALPHA=(J-0.242)/0.20547.00
1447    12   CONTINUE
1448         RETURN
1449         END
```

```
 1470          SUBROUTINE RALPHA (PC,THETA,ALPHA)
 1471 C      ' RIEDEL FACTOR BY MILLER METHOD (VT 3)
 1472          ALPHA=0.9076*(1.+(THETA*ALOG(PC)/(1.-THETA)))
 1473   12     CONTINUE
 1474          RETURN
 1475          END
```

```
 1476        SUBROUTINE RITZ (PO,[illegible],IC,TAUT,IY,NT)
 1477 C      [illegible] VIA OGATA AND TSUCHIDA METHOD
 1478 C             (VOL [illegible])
 1479        DIMENSION PO(20,2),Y(20)
 1480        RITZ=(1X,T,I)*Y([illegible])*PO(IXOT,2)
 1481        RETURN
 1482        END
```

```
 1483          SUBROUTINE RATIO (THETA,VR,TB)
 1484 C        TB BY WATSON'S METHOD (VII 2)
 1485          TB=(THETA/(VR**0.18))*EXP((2.77*VR**0.18)/THETA)\
 1486        1-2.93)
 1487   12     CONTINUE
 1488          RETURN
 1489          END
```

```
1400          SUBROUTINE LYOTS (TH,TA,TC,TS)
1401 C        TH BY LYDERSEN'S METHOD (VI 5)
1402          TH=TS*TA/TC
1403          RETURN
1404          END
```

```
1495           SUBROUTINE STLUP (TC,ZC,PC,ENGY,DIS,RSV,VC,CCDIG,
1496          1COMP)
1497 C         ESTIMATE LENNARD-JONES POTENTIAL PARAMETERS BY STIEL AND
1498 C                 THODOS METHOD (VIII 1)
1499           IF(CCDIG-6.)10,11,10
1500   10      IF(CCDIG-4.)13,12,13
1501   12      DIS=0.9*(VC**0.333)*(ZC**2.75)
1502           ENGY=0.00331*TC/(ZC**4)
1503           RSV=1.2615*DIS**3
1504           GO TO 15
1505   13      DIS=0.785*VC**0.333
1506           ENGY=0.857*TC
1507           RSV=1.2615*DIS**3
1508           GO TO 15
1509   11      ENGY=65.3*TC*(ZC**3.6)
1510           DIS=0.812*((TC/PC)**0.333)/(ZC**0.867)
1511           RSV=(0.076/(ZC**2.6))*(TC/PC)
1512   15      CONTINUE
1513           RETURN
1514           END
```

```
 1515          SUBROUTINE SVB (AVB,VB,GCS)
 1516 C        VOLUME AT THE NORMAL BOILING POINT VIA SCHROEDER'S
 1517 C             METHOD (IX 1)
 1518          DIMENSION AVB(18),GCS(18)
 1519          SUMVB=0.0
 1520          DO 11 N=1,17
 1521       11 SUMVB=SUMVB+AVB(N)*GCS(N)
 1522          VB=SUMVB
 1523          CONTINUE
 1524          RETURN
 1525          END
```

```
 1526           S[illegible] [illegible]ATTER FRAVC (VC,PC,VC)
 1527 C         V[illegible] BRONSON'S METHOD (TX 2)
 1528           VC=VC/(0.422*ALOG10(PC)+1.951)
 1529    12     CONTINUE
 1530           RETURN
 1531           END
```

```
 1532          SUBROUTINE HCAP (TC,T,CPH,XN,XM,RCP,C)
 1533  C    *   COMPUTE GAS HEAT CAPACITY VIA METHOD OF [illegible],
 1534  C               [illegible] AND [illegible] (X 1)
 1535          DIMENSION ACP(20,6),ICARD(20)
 1536          SUMCV=0.0
 1537          SUMCO=0.0
 1538          R=1.987
 1539          DO 11 I=1,20
 1540          C1=ACP(I,1)+ACP(I,2)*T*.001+ACP(I,3)*T*T*0.000001
 1541          SUMCV=SUMCV+C1*ICARD(I)
 1542          C2=ACP(I,4)+ACP(I,5)*T*.001+ACP(I,6)*T*T*0.000001
 1543       11 SUMCO=SUMCO+C2*ICARD(I)
 1544          X=(3.*XN-6.-XM-3)/2
 1545          CPH=4.*R+XM*R/2.+SUMCV+X*SUMCO
 1546          CONTINUE
 1547          RETURN
 1548          END
```

```
1549              SUBROUTINE ACPH ([illegible])
1550 C            THIS HAS HEAT CAPACITY VIA KIRANE AND [illegible]
1551 C                 METHOD (A 2)
1552              DIMENSION RD(47,4),SCRD(46)
1553              SUMA=0.0
1554              SUMB=0.0
1555              SUMC=0.0
1556              SUMD=0.0
1557              DO 10 I=1,46
1558              SUMA=SUMA+RD(I,1)*SCRD(I)
1559              SUMB=SUMB+RD(I,2)*SCRD(I)*.01
1560              SUMC=SUMC+RD(I,3)*SCRD(I)*0.0001
1561          10  SUMD=SUMD+RD(I,4)*SCRD(I)*0.000001
1562              SUMA=SUMA-RD(21,1)*SCRD(11)-RD(5,1)*(SCRD(26)
1563             1+SCRD(29)+SCRD(32)+SCRD(33))
1564              SUMB=SUMB-(RD(21,2)*SCRD(11)-RD(5,2)*(SCRD(26)
1565             1+SCRD(29)+SCRD(32)+SCRD(33)))*0.01
1566              SUMC=SUMC-(RD(21,3)*SCRD(11)-RD(5,3)*(SCRD(26)
1567             1+SCRD(29)+SCRD(32)+SCRD(33)))*0.0001
1568              SUMD=SUMD-(RD(21,4)*SCRD(11)-RD(5,4)*(SCRD(26)
1569             1+SCRD(29)+SCRD(32)+SCRD(33)))*0.000001
1570          12  CP=SUMA+SUMB*T+SUMC*T*T+SUMD*T*T*T
1571              CONTINUE
1572              RETURN
1573              END
```

```
FORTRAN IV G LEVEL  21        [illegible]        SUBROUTINE                     [illegible]/77.      PAGE [illegible]

1574            SUBROUTINE FRNK (TT,FRK,T,TP,N,GCF,GF29)
1575 C          FIND GF FRK AT T VIA FRANKLIN'S METHOD (X, 1)
1576            DIMENSION TT(4),FRK(5,4),GCF(64)
1577            SUMGF=0.0
1578            GF29=0.0
1579            DO 30 K=1,5
1580            IF (T-TT(K))  15,17,16
1581       16   IF(T-TT(5)) 30,50,19
1582       15   IF(K-1) 19,17,21
1583       21   L=K-1
1584            CI=(T-TT(L))/(TT(K)-TT(L))
1585            GO TO 20
1586       17   CI=1.0
1587            L=K
1588       20   DO 49 N=1,64
1589            GF29=GF29+FRK(1,2)*GCF(N)
1590            GF29S=GF29
1591            GY=FRK(1,L)+CI*(FRK(1,K)-FRK(1,L))
1592            SUMGF=SUMGF+GY*GCF(N)
1593            RF=SUMGF
1594       49   CONTINUE
1595            GF29=GF29-FRK(5,2)*(GCF(28)+GCF(31))
1596            GY=FRK(5,L)+CI*(FRK(5,K)-FRK(5,L))
1597            RF=RF-GY*(GCF(28)+GCF(31))
1598            GO TO 100
1599       30   CONTINUE
1600      100   RETURN
1601       19   DO 51 N=1,64
1602            GF29=GF29+FRK(1,2)*GCF(N)
1603       51   RF29=GF29
1604            RF29=RF29-FRK(5,2)*(GCF(28)+GCF(31))
1605            RETURN
1606            END
```

```
 1007           SUBROUTINE VDHF (T,VDHF,FHO,BCVD,VDF,HF298)
 1008 C         HEAT OF FORMATION VIA VERMA AND DORAISWAMY METHOD
 1009 C              (XT 2)
 1010           DIMENSION VD(70,2),BCVD(50),VDH(70),B(70,2)
 1011           TK=T
 1012           SUMVD=0.0
 1013           SUMH=0.0
 1014           VD298=0.0
 1015           H298=0.0
 1016           DO 50 N=1,70
 1017           VD298=VD298+VD(N,1)*BCVD(N)
 1018           H298=H298+HBP(N,1)*BCVD(N)
 1019           TDK=T-298.
 1020           IF(TDK-2.) 15,15,33
 1021       15 TK=300.
 1022       33 IF(TK-300.)  14,16,16
 1023       14 GO TO 15
 1024       16 IF(TK-600.)  17,17,18
 1025       17 SUMVD=SUMVD+VD(N,1)*BCVD(N)
 1026          SUMH=SUMH+HBP(N,1)*BCVD(N)
 1027          GO TO 50
 1028       18 IF(TK-750.) 19,19,20
 1029       19 IF(N-7) 51,21,51
 1030       51 IF(N-30) 52,21,52
 1031       52 IF(N-30) 21,21,53
 1032       53 IF(N-45) 17,21,17
 1033       21 SUMVD=SUMVD+VD(N,2)*BCVD(N)
 1034          SUMH=SUMH+HBP(N,2)*BCVD(N)
 1035          GO TO 50
 1036       20 IF(VDH(N)-1.) 22,22,23
 1037       23 GO TO 15
 1038       22 IF(TK-850.) 24,24,25
 1039       24 IF(N-9) 17,17,54
 1040       54 IF(N-29) 55,17,56
 1041       55 IF(N-20) 56,17,17
 1042       56 IF(N-59) 21,21,17
 1043       25 IF(TK-1000.) 26,26,27
 1044       26 IF(N-4) 21,26,21
 1045       28 IF(TK-1100.) 17,17,21
 1046       27 IF(TK-1500.) 28,28,50
 1047       10 GO TO 15
 1048       25 IF(VDF(N)) 61,21,15
 1049       50 CONTINUE
 1050           H298=H298-HB(7,1)*(BCVD(26)+BCVD(23)+BCVD(24)
 1051         1+BCVD(27)+BCVD(28))-VD(7,1)*(BCVD(27)+BCVD(3[illegible]
 1052         2+BCVD(29))
 1053           VD298=VD298-VD(7,1)*(BCVD(30)+BCVD(23)+BCVD(24)
 1054         1+BCVD(27)+BCVD(28))-VD(7,1)*(BCVD(27)+BCVD(3[illegible]
 1055         2+BCVD(29))
 1056       64 HF298=VD298+H298*[illegible].01
```

```
1057          IF(M-39) 100,100,200
1058     100  SUMB=SUMB - B(7,1)*(BCVB(20)+BCVB(23)+BCVB(24)
1059         1+BCVB(27)+BCVB(28))-VB(8,1)*(BCVB(27)+BCVB(28)
1060         2+BCVB(29))
1061          SUMVB=SUMVB-VB(7,1)*(BCVB(20)+BCVB(23)+BCVB(24)
1062         1+BCVB(27)+BCVB(28))-VB(8,1)*(BCVB(27)+BCVB(28)
1063         2+BCVB(29))
1064          GO TO 300
1065     200  SUMB=SUMB-B(7,2)*(BCVB(20)+BCVB(23)+BCVB(24)
1066         1+BCVB(27)+BCVB(28))-VB(8,2)*(BCVB(27)+BCVB(28)
1067         2+BCVB(29))
1068          SUMVB=SUMVB-VB(7,2)*(BCVB(20)+BCVB(23)+BCVB(24)
1069         1+BCVB(27)+BCVB(28))-VB(8,2)*(BCVB(27)+BCVB(28)
1070         2+BCVB(29))
1071     300  CONTINUE
1072          HT=SUMVB+SUMB*TK*.01
1073          GO TO 61
1074      15  IF(M-79) 60,60,65
1075      60  DO 62 N=1,79
1076          VB29B=VB29B+VB(N,1)*BCVB(N)
1077      62  B29B=B29B+B(N,1)*BCVB(N)
1078          B29B=B29B-B(7,1)*(BCVB(20)+BCVB(23)+BCVB(24)
1079         1+BCVB(27)+BCVB(28))-VB(8,1)*(BCVB(27)+BCVB(28)
1080         2+BCVB(29))
1081          VB29B=VB29B-VB(7,1)*(BCVB(20)+BCVB(23)+BCVB(24)
1082         1+BCVB(27)+BCVB(28))-VB(8,1)*(BCVB(27)+BCVB(28)
1083         2+BCVB(29))
1084          HF29A=VB29B+B29B*294.*.01
1085          GO TO 69
1086      61  RETURN
1087      65  RETURN 1
1088          END
```

```
1069          SUBROUTINE [illegible] ([illegible],HF,CGL,[illegible]20)
1070 C        HEAT OF FORMATION VIA BOND ENERGY METHOD (XI B)
1071          DIMENSION BE(40),CGL(40)
1072          SUMGL=0.0
1073          DO 11 I=1,39
1074      11  SUMGL=SUMGL+BE(I)*CGL(I)
1075      13  HF=SUMGL
1076          [illegible]
1077      15  CONTINUE
1078          RETURN
1079          END
```

```
 1700          SUBROUTINE A[illegible] ([illegible],AAAE,ARS,AF,FRT,GCABW,FCABW,[illegible],
 1701 C        DENSITY AND [illegible] [illegible] OF [illegible] BY [illegible]
 1702 C                [illegible] [illegible] [illegible] (XII [illegible])
 1703           DIMENSION AAAE(14),ARS(58),GCABW(30),FCABW(15)
 1704           F=1.208
 1705          SUMS=0.0
 1706          SUM=0.0
 1707          K=0.0
 1708       10 K=K+1
 1709          IF(GCABW(K)-50.) 11,12,40
 1710       11 IF(GCABW(K)-40.) 14,15,15
 1711       15 IF(GCABW(K)-51.) 16,16,14
 1712       14 I=GCABW(K)
 1713          SUMS=SUMS+ARS(I)
 1714          GO TO 10
 1715       16 I=GCABW(K)
 1716          SUMS=SUMS+ARS(I)*1.0
 1717          GO TO 10
 1718       12 SUM=SUMS
 1719          DO 20 J=1,15
 1720       20 SUM=SUM-FCABW(J)*AAAAE(J)
 1721          EF=SUM
 1722          SEF=EF-T*EF/1000.
 1723       40 CONTINUE
 1724          RETURN
 1725          END
```

```
 1726           SUBROUTINE [illegible] (I,T,ENGY,DTS,UO)
 1727 C         LOW PRESSURE VISCOSITY BY THEORETICAL METHOD
 1728 C                  (NOTE 1)
 1729           [illegible]=1/ENGY
 1730           CI=1./(0.6077*(1.+0.7207*ALOG(TS(NR))))
 1731           UO=0.0026693*SQRT(WT*T)/(DIS*DIS*CI)
 1732   11      GO TO 99
 1733           ENTRY T[illegible] (TS,T,ENGY,DIS,CIV,TS,D,DIPOLE,UO,W,
 1734          1T,DELTA)
 1735           DIMENSION CIV(37,8),TS(37),D(8)
 1736           [illegible]=DIPOLE
 1737           TSTAR=T/ENGY
 1738           DELTA=(D*D*DM*DIS/10.**8.)*(DIS*DIS*ENGY*1.38053/
 1739          1(10.**23.)
 1740           DO 20 I=1,37
 1741           IF(TSTAR-TS(I))12,13,13
 1742   12      IF(I-1)14,14,15
 1743   14      RETURN 1
 1744   15      IF(I-37)16,16,17
 1745   [illegible]      RETURN 2
 1746   17      RETURN 1
 1747   13      IF(TSTAR-TS(I+1))16,20,20
 1748   20      CONTINUE
 1749   16      X=TSTAR-TS(I)
 1750           Y=TS(I+1)-TS(I)
 1751           FRACT=X/Y
 1752           DO 30 J=1,8
 1753           IF(DELTA-D(J))21,22,22
 1754   21      IF(J-1)23,23,24
 1755   23      RETURN 3
 1756   24      IF(J-8)25,25,26
 1757   25      RETURN 2
 1758   26      RETURN [illegible]
 1759   22      IF(DELTA-D(J+1))27,30,30
 1760   30      CONTINUE
 1761   27      X=DELTA-D(J)
 1762           Y=D(J+1)-D(J)
 1763           FACT=X/Y
 1764           CI1=CIV(I,J)+FRACT*(ABS(CIV(I,J)-CIV(I+1,J)))
 1765           CI2=CIV(I,J+1)-FRACT*(ABS(CIV(I,J+1)-CIV(I+1,J+1)))
 1766           IF(CI1-CI2)31,32,33
 1767   31      CI=CI1+FACT*(ABS(CI2-CI1))
 1768           GO TO 75
 1769   32      CI=CI1
 1770           GO TO 75
 1771   33      CI=CI1-FACT*(ABS(CI2-CI1))
 1772   75      UO=0.0026693*SQRT(WT*T)/(DIS*DIS*CI)
 1773   99      CONTINUE
 1774           RETURN
 1775           END
```

```
 1776          SUBROUTINE [illegible] (T,WT,TC,PC,ZC,UO,*,*,MWR)
 1777 C        LOW PRESSURE VISCOSITY BY STIEL AND THODOS METHOD
 1778 C            (REID P)
 1779          E=(TC**0.167)/(SQRT(WT)*(PC**0.667))
 1780          TR=T/TC
 1781          IF(TR-1.5)10,10,11
 1782    10    UO=(0.00034/E)*(TR**0.94)
 1783          GO TO 12
 1784    11    UO=(0.0001776/E)*((4.58*TR-1.67)**0.625)
 1785    12    GO TO 60
 1786          ENTRY [illegible] (T,WT,TC,PC,ZC,UO,*,*,MWR)
 1787          E=(TC**0.167)/(SQRT(WT)*(PC**0.667))
 1788          TR=T/TC
 1789          IF(TR-2.0)13,13,14
 1790    13    RETURN 1
 1791    14    UO=((7.55*TR-0.55)*0.00001/E)*1./(ZC**1.25)
 1792          GO TO 60
 1793          ENTRY [illegible] (T,WT,TC,PC,ZC,UO,*,*,MWR)
 1794          E=(TC**0.167)/(SQRT(WT)*(PC**0.667))
 1795          TR=T/TC
 1796          IF(TR-2.5)15,15,16
 1797    15    RETURN 1
 1798    16    UO=((1.90*TR-0.29)*0.0001/E)*1./(ZC**0.667)
 1799    60    CONTINUE
 1800          RETURN
 1801          END
```

```
1802          [illegible] (T,[illegible],V,S,SY,HSV,U)
1803 C        HIGH PRESSURE VISCOSITY BY CURRMANS AND [illegible]
1804 C               METHOD (XIV )
1805          [illegible]SV/[illegible]
1806          [illegible]=[illegible]/[illegible]Y
1807          [illegible]=(0.35*[illegible]*0.6*[illegible]*0.61*[illegible](  ))
1808         1/([illegible]**0.94))
1809    12    CONTINUE
1810          RETURN
1811          END
```

```
1812          SUBROUTINE JOSTD1 (TC,PC,VC,V,U0,WT,U,*,RHOR)
1813 C        [illegible] VISCOSITY BY JOSSI, STIEL AND THODOS
1814 C               [illegible] (XIV-2)
1815          E=(TC**0.167)/(SQRT(WT)*(PC**0.667))
1816          RHOR=VC/V
1817          A=0.1023+0.023364*RHOR+0.058533*RHOR*RHOR-0.0407
1818         1[illegible]*RHOR*RHOR+0.0093324*RHOR*RHOR*RHOR*RHOR
1819          U=((A*A*A*A-0.0001)/E)+U0
1820    11    GO TO 99
1821          ENTRY JOSTD2 (TC,PC,VC,V,U0,WT,U,*,RHOR)
1822          E=(TC**0.167)/(SQRT(WT)*(PC**0.667))
1823          RHOR=VC/V
1824          IF(RHOR-2.2)12,12,13
1825    12    DEL=0.
1826          GO TO 98
1827    13    DEL=0.0004750*(RHOR*RHOR*RHOR-10.65)*(RHOR*RHOR*
1828         1RHOR-10.65)
1829    98    IF(RHOR-0.1)14,15,15
1830    14    U=(0.00001656*(RHOR**1.111)/E)+U0
1831          GO TO 99
1832    15    IF(RHOR-0.9)16,16,17
1833    16    U=(0.00000607*((9.045*RHOR+0.63)**1.739)/E)+U0
1834          GO TO 99
1835    17    IF(RHOR-2.6)18,19,19
1836    18    X=0.6439-0.1005*RHOR-DEL
1837          Y=10.**X
1838          Y=4.-Y
1839          Z=10.**Y
1840          U=(Z/E)+U0
1841          GO TO 99
1842    19    IF(RHOR-2.8)20,20,21
1843    20    U=(0.00090/E)+U0
1844          GO TO 99
1845    21    IF(RHOR-3.0)22,22,23
1846    22    U=(0.0025/E)+U0
1847          GO TO 99
1848    23    RETURN 1
1849    99    CONTINUE
1850          RETURN
1851          END
```

```
              [illegible] (12),CV(12),[illegible] 
         1 [illegible] (12)
      C       [illegible] CONDUCTIVITY BY [illegible]
      C                [illegible] ( [illegible] )
              [illegible] (12),ACB(12)
              [illegible] -1.) /[illegible]
            [illegible] -*CV*2.5+.01/.T
              [illegible]
            [illegible] R-2.) [illegible]
            [illegible] =./TC
              [illegible] =1*(1.50*CV+2.4-0.7/TR)*.01/ST
              [illegible]
            [illegible] =../VO
              [illegible] =1,[illegible]7
              TR=1/TC
              SV=[illegible]V./18
              [illegible] =5.0*RHO*(SV-3.75-R*ALOG(TD))
              [illegible] =1/.00.
              [illegible] =1-[illegible]
              SUMCI=0.0
              DO 20 L=1,12
         20   SUMCI=SUMCI+(CIREF(J,L)+(T/100.-I)*(CIREF(J,L)-CIREF([illegible])))
              [illegible] (L)
              [illegible] =[illegible]*(1.50*CV+5.60-0.5*SUMCI-0.39/TR-0.*ALPHA)*
            1 [illegible] /ST
         10   CONTINUE
              RETURN
              END
```

```
1880          SUBROUTINE STR (ZC,TC,PC,V,W1,TRC,[illegible],THC,[illegible])
1881 C        THIS SUBROUTINE CALCULATES THE THERMAL CONDUCTIVITY BY STIEL AND
1882 C              THODOS METHOD (RV 2)
1883          X=(TC**0.167)*SQRT(W1)/(PC**0.667)
1884          VC=(82.05*ZC*TC)/PC
1885          RHOR=VC/V
1886          [illegible]-7.*ALOG10(TR)
1887          IF(RHOR-0.5)10,10,11
1888    10    THC=(0.0000014*(1./EXP(0.535*RHOR)-1.)/(X*ZC**5)
1889         1)+THCO
1890          GO TO 17
1891    11    IF(RHOR-2.0)12,12,13
1892    12    THC=(0.0000013)*(EXP(0.67*RHOR)-1.069)/(X*ZC**5)
1893         1)+THCO
1894          GO TO 17
1895    13    IF(RHOR-2.8)14,14,15
1896    14    THC=(0.0000000002976*(EXP(1.155*RHOR)+2.016)/(X*ZC**
1897         15))+THCO
1898          GO TO 17
1899    15    RETURN 1
1900    17    CONTINUE
1901          RETURN
1902          END
```

```
1903          SUBROUTINE [illegible] (P,TC,TR,HVC,EVA)
1904 C        ENTHALPY AND [illegible] OF VAPORIZATION AT TR BY
1905 C              RIEDEL-PLANCK-MILLER EQUATION (XVI 1)
1906          [illegible]=1.-[illegible]
1907          [illegible]
1908          H=(TBR*ALOG(PC))/(1.-TBR)
1909          G=.4835+0.4605*H
1910          [illegible]=1.-0.97/([illegible])
1911          AK=[illegible]/(2.303*G)-(1.+TBR)
1912          HVC=2.303*G*R*TC*ZVC*(1.*TR*TR+AK*(1.+2.*TR))
1913          EVA=HVC/TB
1914   10     CONTINUE
1915          RETURN
1916          END
```

```
1917          SUBROUTINE SATVP (T,ETC,TC,TB,ALPHA,VP)
1918 C        VAPOR PRESSURE BY RIEDEL METHOD OR RIEDEL-PLANK-
1919 C               MILLER METHOD (EQUT 1 AND 2)
1920          TR=T/TC
1921          PHI=-35.+36./TR+42.*ALOG(TR)-TR**6
1922          A2=0.0838*(3.758-ALOG10(TR))
1923          PVR=.118*PHI-7.*ALOG10(TR)
1924          PVR=PVR-A1-(ALPHA-7.)*A2
1925          VPR=10.**PVPR
1926          VP=VPR*PC
1927          IF(VP-1.275)5,5,6
1928    6     TBR=TB/TC
1929          H=TBR*(ALOG10(PC)/(1.-TBR))
1930          G=0.227+0.4325*H
1931          K=(H/G-(1.+TBR))/((1.-TBR)*(1.-TBR))
1932          TR=T/TC
1933          PVPR=-(G/TR)*(1.-TR*TR+K*(1.-TR)**3)
1934          VPR=10.**PVPR
1935          VP=VPR*PC
1936    5     CONTINUE
1937          RETURN
1938          END
```

```
1939          SUBROUTINE RKZ (T,P,Z,V,RHO,DEL,S,PHC,H,Z1,Z2,
1940        * Z3,TC,PC)
1941 C        SOLUTION OF REDLICH-KWONG EQUATION FOR Z. THE
1942 C                 EQUATION IS  Z**3-Z**2+((P*A/(R*R*T**2.5))-
1943 C                 (P*P*B*B/(R*R*T*T))-(B*P/(R*T)))*Z-P*P*A*B/
1944 C                 (R*R*R*T**3.5)=0
1945 C        SEE CRC BOOK FOR SOLUTION OF CUBIC EQUATION
1946          R=82.056
1947          PI=3.1415927
1948          A=0.4278*R*R*TC**2.5/PC
1949          B=0.0867*R*TC/PC
1950          C1=P*A/(R*R*T**2.5)-P*P*B*B/(R*R*T*T)-B*P/(R*T)
1951          C0=-P*P*A*B/(R*R*R*T**3.5)
1952          C=1./3.
1953          ALPHA=C1-C
1954          BETA=C0+C1/3.-2./27.
1955          TAU=BETA*BETA/4.+ALPHA*ALPHA*ALPHA/27.
1956          IF(TAU)10,11,12
1957 C        ONE REAL ROOT
1958    12    Z=((-BETA/2.+SQRT(TAU))**C)+((-BETA/2.-SQRT(TAU)
1959         )**C)+C
1960          GO TO 99
1961 C        THREE REAL ROOTS, AT LEAST TWO OF WHICH ARE EQUAL
1962    11    Z1=-((-BETA/2.)**C)+C
1963          Z2=((-BETA/2.)**C)+C
1964          IF(Z1)20,20,30
1965    20    IF(Z2-.5)31,31,33
1966    31    Z=Z2
1967          GO TO 99
1968    30    IF(Z1-.5)32,32,20
1969    32    Z=Z1
1970          GO TO 99
1971    33    Z3=0.
1972          GO TO 22
1973 C        THREE REAL AND UNEQUAL ROOTS
1974    10    OMEGA=SQRT(((BETA*BETA)/4.)/((-ALPHA**3)/27.))
1975          THETA=ATAN(SQRT((1./OMEGA)*(1./OMEGA)-1.))
1976          IF(BETA)13,14,14
1977    13    THETA=PI-THETA
1978    14    IF(ALPHA)15,15,16
1979    15    F=2.
1980          GO TO 17
1981    16    F=-2.
1982    17    Z1=F*SQRT(-ALPHA/3.)*COS(THETA/3.)+C
1983          Z2=F*SQRT(-ALPHA/3.)*COS(THETA/3.+2.*PI/3.)+C
1984          Z3=F*SQRT(-ALPHA/3.)*COS(THETA/3.+4.*PI/3.)+C
1985          IF(Z1)18,18,19
1986    19    IF(Z1-.5)25,18,18
1987    18    IF(Z2)21,21,22
1988    22    IF(Z2-.5)26,21,21
```

```
1989   21    IF(Z-1)22,23,24
1990   24    IF(Z-5.)27,22,22
1991   22    RETURN 1
1992   23    Z=1.
1993         GO TO 99
1994   26    Z=5.
1995         GO TO 99
1996   27    B=Z3
1997   99    CONTINUE
1998         V=V*R*T/P
1999         VELN=1.957*T-P*V*0.0241173+(3.*A*0.0242173/(2.*B*
2000        1SQRT(T)))*ALOG((V+B)/V)
2001         SCLS=1.987*ALOG(1./Z)+1.987*ALOG(V/(V-B))+(A*
2002        10.0242173/(2.*B*T**1.5))*ALOG((V+B)/V)
2003         FUG=1./Z-1.-ALOG((P/(R*T))*(V-B))-(A/(B*R*T**1.5)
2004        1)*ALOG(1.+B/V)
2005         FUGC=2.71828**FUG
2006         RETURN
2007         END
```

```
2008          SUBROUTINE RKCP (T,V,TC,PC,CPO,CP)
2009 C **     CP BY USE OF R-K EQUATION OF STATE  (XIX 1)
2010          R=82.050
2011          TR=T/TC
2012          B=.0867*R*TC/PC
2013          CP=CPO+(5.*0.427*1.987/(4.*0.0867*TR**1.5))*ALOG(
2014         1(1.+0.0867/PC)/TR)+3.*0.427*1.987/(2.*PC*TR**2.5
2015         2*4.*0.0867*TR**1.5)
2016          RETURN
2017          END
```

```
 2018                SUBROUTINE RKCV (T,V,TC,PC,VC,CP,CV)
 2019 C         CV BY USE OF R-K EQUATION OF STATE  (XX [illegible])
 2020           R= [illegible]
 2021           VR=V/VC
 2022           B=0.0867*R*TC/PC
 2023           TR=T/TC
 2024           ZC=PC*VC/(R*TC)
 2025           A=(0.42/(Z*R *R*TC**2.5)/PC
 2026           [illegible]-VC/V
 2027           XX=[illegible]*R*TC/(PC*(VC-[illegible]))+A*RHO[illegible]/(2.*PC
 2028          1*VC*(VC+B*RHO[illegible])*SQRT(TC)*TR**1.5)
 2029           YYY=A*B*VC/(PC*(VC-B*RHO[illegible])*(VC-B*RHO[illegible]))-(2.*VC+B*
 2030          1[illegible])*A*RHO[illegible]/(SQRT(T)*PC*VC*(VC+B*RHO[illegible])*(VC+B*
 2031          2[illegible]))
 2032           CV=CP-1.987*ZC*TR*XX*XX/(RHO*RHO*YYY)
 2033           RETURN
 2034           END
```

```
                THE ESTIMATED PHYSICAL PROPERTIESOF

                           ACETYLENE

        T= 373.00 DEG K       P=    1.00 ATM      MOLE WT= 26.04

        373.00       DEG K,             T

          1.00       ATM,               P

      30510.50       CC/G MOLE,         V

          0.997                         Z

        178.46       DEG K,             NORMAL BOILING PT.

         46.24       CC/G MOLE,         VOLUME AT NORMAL BOILING
                                                POINT

        309.35       DEG K,             TC

         62.40       ATM,               PC

        126.64       CC/G MOLE,         VC

          0.311                         ZC

        204.824      ATM,               VAPOR PRESSURE

          6.04                          RIEDEL FACTOR

          0.046                         ACENTRIC FACTOR

         11.551      CAL/G MOLE-DEG K,  CPO

         11.570      CAL/G MOLE-DEG K,  CP

          9.557      CAL/G MOLE-DEG K,  CV

        302.56       DEG K,             E/K

          3.806      ANGSTROMS,         INTERMOLECULAR DISTANCE

         69.66       CC/G MOLE,         HARD-SPHERE VOLUME

          0.01351    CENTIPOISE,        VISCOSITY AT LOW PRESSURE

          0.01353    CENTIPOISE,        VISCOSITY AT ELEVATED
                                                PRESSURE

          0.0000792  CAL/CM-SEC-DEG K,  THERMAL CONDUCTIVITY AT
                                                LOW PRESSURE
```

```
      0.0000791  CAL/CM-SEC-DEG K, THERMAL CONDUCTIVITY AT
                                            ELEVATED PRESSURE

      7.05       CAL/G MOLE,       H(IDEAL)-H(IDEAL)-H(REAL)

      0.013      CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

      1.003                        FUGACITY COEFFICIENT

   3410.3        CAL/G MOLE,       HEAT OF VAPORIZATION
                                            AT NORMAL BOILING PT.

     19.109      CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                            AT NORMAL BOILING PT.

     54.156      KCAL/G MOLE,      HEAT OF FORMATION AT
                                            STATED TEMPERATURE

     54.200      KCAL/G MOLE,      HEAT OF FORMATION FOR
                                            IDEAL GAS AT 1 ATM
                                            AND 298 DEG K

     14.167      CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                            IDEAL GAS AT 1 ATM
                                            AND 298 DEG K.

     48.916      KCAL/G MOLE,      FREE ENERGY OF FORMATION
                                            FOR IDEAL GAS AT 1
                                            ATM AND 298 DEG K.
```

```
  LIQUID PHYSICAL PROPERTIES

 T=153.000000 DEG-K       P=  1.000000 ATM

     0.5264       GRAMS/CC             LIQUID DENSITY

 SATURATED LIQUID ENTHALPY CALC
 -3438.9968       CAL/G MOLE           LIQ. ENTHALPY DEPARTURE

 REDUCED DENSITY>2.0 FOR BWR METHOD
 REDUCED TEMPERATURE<0.6 FOR BWR METHOD
     5.2601       CAL/G MOLE-C         HT CAPACITY DEPARTURE

 VISCOSITY CANNOT BE CALCULATED-NO INPUT DATA
    49.6000       (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

  -873.9082       CAL/G MOLE-K         LIQ ENTROPY DEPARTURE

   1.007961       DYNES/CM             SURFACE TENSION

   0.001692       1/DEG K              COEFF OF THRMAL EXP
```

```
                THE ESTIMATED PHYSICAL PROPERTIESOF

                              ANALINE

        T= 473.00 DEG K       P=    1.00 ATM      MOLE WT= 93.12

        473.00       DEG K,              T

          1.00       ATM,                P

      38118.68       CC/G MOLE,          V

          0.982                          Z

        436.62       DEG K,              NORMAL BOILING PT.

         98.17       CC/G MOLE,          VOLUME AT NORMAL BOILING
                                                 POINT

        667.01       DEG K,              TC

         50.42       ATM,                PC

        265.00       CC/G MOLE,          VC

          0.244                          ZC

          2.474      ATM,                VAPOR PRESSURE

          7.63                           RIEDEL FACTOR

          0.370                          ACENTRIC FACTOR

         37.868      CAL/G MOLE-DEG K,   CPO

         37.958      CAL/G MOLE-DEG K,   CP

         35.845      CAL/G MOLE-DEG K,   CV

          1.440      DEBYES,             DIPOLE MOMENT

        598.31       DEG K,              E/K

          5.033      ANGSTROMS,          INTERMOLECULAR DISTANCE

        160.81       CC/G MOLE,          HARD-SPHERE VOLUME

          0.01227    CENTIPOISE,         VISCOSITY AT LOW PRESSURE

          0.01230    CENTIPOISE,         VISCOSITY AT ELEVATED
                                                 PRESSURE

          0.0000606  CAL/CM-SEC-DEG K,   THERMAL CONDUCTIVITY AT
                                                 LOW PRESSURE
```

```
      METHOD FOR K NOT APPLICABLE

           45.44      CAL/G MOLE,            H(IDEAL)-H(IDEAL)-H(REAL)

           0.061      CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

           1.019                             FUGACITY COEFFICIENT

         9971.7       CAL/G MOLE,            HEAT OF VAPORIZATION
                                                  AT NORMAL BOILING PT.

          22.839      CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                                  AT NORMAL BOILING PT.

          19.649      KCAL/G MOLE,           HEAT OF FORMATION AT
                                                  STATED TEMPERATURE

          21.270      KCAL/G MOLE,           HEAT OF FORMATION FOR
                                                  IDEAL GAS AT 1 ATM
                                                  AND 298 DEG K

         -68.688      CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                                  IDEAL GAS AT 1 ATM
                                                  AND 298 DEG K.

          53.759      KCAL/G MOLE,           FREE ENERGY OF FORMATION
                                                  FOR IDEAL GAS AT 1
                                                  ATM AND 298 DEG K.
```

```
LIQUID PHYSICAL PROPERTIES

T=293.000000 DEG-K        P=  1.000000 ATM

     1.1171       GRAMS/CC            LIQUID DENSITY

SATURATED LIQUID ENTHALPY CALC
-5219.3242        CAL/G MOLE          LIQ. ENTHALPY DEPARTURE

REDUCED DENSITY>2.0 FOR BWR METHOD
REDUCED TEMPERATURE<0.6 FOR BWR METHOD
     7.8855       CAL/G MOLE-C        HT CAPACITY DEPARTURE

     3.1699       CENTIPOISE          LIQ VISCOSITY

   202.0996       (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

     0.1306       CAL/G MOLE-K        LIQ ENTROPY DEPARTURE

  34.538574       DYNES/CM            SURFACE TENSION

   0.000968       1/DEG K             COEFF OF THRMAL EXP
```

```
                THE ESTIMATED PHYSICAL PROPERTIESOF

                              BENZENE

           T= 373.00 DEG K       P=    1.00 ATM      MOLE WT= 78.11

         373.00       DEG K,                  T

           1.00       ATM,                    P

       29768.30       CC/G MOLE,              V

           0.973                              Z

         381.95       DEG K,                  NORMAL BOILING PT.

         104.18       CC/G MOLE,              VOLUME AT NORMAL BOILING
                                                   POINT

         507.58       DEG K,                  TC

          48.89       ATM,                    PC

         280.64       CC/G MOLE,              VC

           0.275                              ZC

           0.768      ATM,                    VAPOR PRESSURE

           6.86                               RIEDEL FACTOR

           0.215                              ACENTRIC FACTOR

          24.744      CAL/G MOLE-DEG K,       CPO

          24.877      CAL/G MOLE-DEG K,       CP

          22.697      CAL/G MOLE-DEG K,       CV

         381.29       DEG K,                  E/K

           5.752      ANGSTROMS,              INTERMOLECULAR DISTANCE

         240.58       CC/G MOLE,              HARD-SPHERE VOLUME

           0.00953    CENTIPOISE,             VISCOSITY AT LOW PRESSURE

           0.00996    CENTIPOISE,             VISCOSITY AT ELEVATED
                                                   PRESSURE

           0.0000364  CAL/CM-SEC-DEG K,       THERMAL CONDUCTIVITY AT
                                                   LOW PRESSURE
```

```
      0.0000362  CAL/CM-SEC-DEG K, THERMAL CONDUCTIVITY AT
                                           ELEVATED PRESSURE

     54.06          CAL/G MOLE,        H(IDEAL)-H(IDEAL)-H(REAL)

      0.091      CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

      1.029                            FUGACITY COEFFICIENT

   7912.5           CAL/G MOLE,        HEAT OF VAPORIZATION
                                           AT NORMAL BOILING PT.

     20.716      CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                           AT NORMAL BOILING PT.

     18.874         KCAL/G MOLE,       HEAT OF FORMATION AT
                                           STATED TEMPERATURE

     19.800         KCAL/G MOLE,       HEAT OF FORMATION FOR
                                           IDEAL GAS AT 1 ATM
                                           AND 298 DEG K

    -37.399      CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                           IDEAL GAS AT 1 ATM
                                           AND 298 DEG K.

     33.750         KCAL/G MOLE,       FREE ENERGY OF FORMATION
                                           FOR IDEAL GAS AT 1
                                           ATM AND 298 DEG K.
```

```
LIQUID PHYSICAL PROPERTIES

T=293.000000 DEG-K       P=  1.000000 ATM

     0.8028       GRAMS/CC              LIQUID DENSITY

SATURATED LIQUID ENTHALPY CALC
-3884.5286        CAL/G MOLE            LIQ. ENTHALPY DEPARTURE

REDUCED DENSITY>2.0 FOR BWR METHOD
REDUCED TEMPERATURE<0.6 FOR BWR METHOD
     5.0318       CAL/G MOLE-C          HT CAPACITY DEPARTURE

     0.6063       CENTIPOISE            LIQ VISCOSITY

   148.7998       (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

  -285.3557       CAL/G MOLE-K          LIQ ENTROPY DEPARTURE

   5.466660       DYNES/CM              SURFACE TENSION

   0.001081       1/DEG K               COEFF OF THRMAL EXP
```

```
                   THE ESTIMATED PHYSICAL PROPERTIESOF

                               ACETIC ACID

           T= 373.00 DEG K      P=   0.50 ATM      MOLE WT= 60.05

           373.00        DEG K,             T

             0.50        ATM,               P

         60622.52        CC/G MOLE,         V

             0.990                          Z

           392.52        DEG K,             NORMAL BOILING PT.

            67.69        CC/G MOLE,         VOLUME AT NORMAL BOILING
                                                     POINT

           593.84        DEG K,             TC

            64.22        ATM,               PC

           185.72        CC/G MOLE,         VC

             0.245                          ZC

             0.499       ATM,               VAPOR PRESSURE

             8.24                           RIEDEL FACTOR

             0.495                          ACENTRIC FACTOR

            13.600       CAL/G MOLE-DEG K,  CPO

            18.695       CAL/G MOLE-DEG K,  CP

            16.642       CAL/G MOLE-DEG K,  CV

             1.440       DEBYES,            DIPOLE MOMENT

           547.66        DEG K,             E/K

             4.381       ANGSTROMS,         INTERMOLECULAR DISTANCE

           106.10        CC/G MOLE,         HARD-SPHERE VOLUME

             0.01043     CENTIPOISE,        VISCOSITY AT LOW PRESSURE

             0.01044     CENTIPOISE,        VISCOSITY AT ELEVATED
                                                     PRESSURE

             0.0000395   CAL/CM-SEC-DEG K,  THERMAL CONDUCTIVITY AT
                                                     LOW PRESSURE
```

```
METHOD FOR K NOT APPLICABLE

      19.04        CAL/G MOLE,           H(IDEAL)-H(IDEAL)-H(REAL)

      0.032        CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

      1.010                              FUGACITY COEFFICIENT

    9691.7         CAL/G MOLE,           HEAT OF VAPORIZATION
                                              AT NORMAL BOILING PT.

     25.201        CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                              AT NORMAL BOILING PT.

   -104.713        KCAL/G MOLE,          HEAT OF FORMATION AT
                                              STATED TEMPERATURE

   -104.720        KCAL/G MOLE,          HEAT OF FORMATION FOR
                                              IDEAL GAS AT 1 ATM
                                              AND 298 DEG K

    -34.047        CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                              IDEAL GAS AT 1 ATM
                                              AND 298 DEG K.

    -92.020        KCAL/G MOLE,          FREE ENERGY OF FORMATION
                                              FOR IDEAL GAS AT 1
                                              ATM AND 298 DEG K.
```

```
 LIQUID PHYSICAL PROPERTIES


 T=293.000000 DEG-K        P=  1.000000 ATM

     1.0825        GRAMS/CC             LIQUID DENSITY

 SATURATED LIQUID ENTHALPY CALC
 -4684.5430        CAL/G MOLE           LIQ. ENTHALPY DEPARTURE

 REDUCED DENSITY>2.0 FOR BWR METHOD
 REDUCED TEMPERATURE<0.6 FOR BWR METHOD
     7.2906        CAL/G MOLE-C         HT CAPACITY DEPARTURE

     1.2721        CENTIPOISE           LIQ VISCOSITY

   114.3999        (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

   -33.3943        CAL/G MOLE-K         LIQ ENTROPY DEPARTURE

  16.080109        DYNES/CM             SURFACE TENSION

   0.001110        1/DEG K              COEFF OF THRMAL EXP
```

```
                THE ESTIMATED PHYSICAL PROPERTIESOF

                            ACETIC ANHYDRIDE

       T= 473.00 DEG K      P=  10.00 ATM      MOLE WT=102.09

       473.00       DEG K,              T

        10.00       ATM,                P

      3206.85       CC/G MOLE,          V

         0.826                          Z

       409.07       DEG K,              NORMAL BOILING PT.

       102.57       CC/G MOLE,          VOLUME AT NORMAL BOILING
                                                  POINT

       594.48       DEG K,              TC

        43.38       ATM,                PC

       274.05       CC/G MOLE,          VC

         0.244                          ZC

         5.333      ATM,                VAPOR PRESSURE

         8.48                           RIEDEL FACTOR

         0.543                          ACENTRIC FACTOR

        34.592      CAL/G MOLE-DEG K,   CPO

        34.670      CAL/G MOLE-DEG K,   CP

        30.797      CAL/G MOLE-DEG K,   CV

         1.440      DEBYES,             DIPOLE MOMENT

       533.25       DEG K,              E/K

         5.089      ANGSTRUMS,          INTERMOLECULAR DISTANCE

       166.30       CC/G MOLE,          HARD-SPHERE VOLUME

         0.01335    CENTIPOISE,         VISCOSITY AT LOW PRESSURE

         0.01381    CENTIPOISE,         VISCOSITY AT ELEVATED
                                                  PRESSURE

         0.0000564  CAL/CM-SEC-DEG K,   THERMAL CONDUCTIVITY AT
                                                  LOW PRESSURE
```

```
        METHOD FOR K NOT APPLICABLE

             456.77       CAL/G MOLE,          H(IDEAL)-H(IDEAL)-H(REAL)

              0.647       CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

              1.251                            FUGACITY COEFFICIENT

           10021.0        CAL/G MOLE,          HEAT OF VAPORIZATION
                                                   AT NORMAL BOILING PT.

             24.497       CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                                   AT NORMAL BOILING PT.

           -124.765       KCAL/G MOLE,         HEAT OF FORMATION AT
                                                   STATED TEMPERATURE

           -122.840       KCAL/G MOLE,         HEAT OF FORMATION FOR
                                                   IDEAL GAS AT 1 ATM
                                                   AND 298 DEG K

             -4.422       CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                                   IDEAL GAS AT 1 ATM
                                                   AND 298 DEG K.

             21.029       KCAL/G MOLE,         FREE ENERGY OF FORMATION
                                                   FOR IDEAL GAS AT 1
                                                   ATM AND 298 DEG K.
```

```
,LIQUID PHYSICAL PROPERTIES

T=293.000000 DEG-K        P=  1.000000 ATM

     1.1495       GRAMS/CC             LIQUID DENSITY

SATURATED LIQUID ENTHALPY CALC
-4614.3867        CAL/G MOLE           LIQ. ENTHALPY DEPARTURE

REDUCED DENSITY>2.0 FOR BWR METHOD
REDUCED TEMPERATURE<0.6 FOR BWR METHOD
     4.6930       CAL/G MOLE-C         HT CAPACITY DEPARTURE

     1.0090       CENTIPOISE           LIQ VISCOSITY

   181.1997       (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

    -2.6000       CAL/G MOLE-K         LIQ ENTROPY DEPARTURE

  17.318085       DYNES/CM             SURFACE TENSION

   0.001111       1/DEG K              COEFF OF THRMAL EXP
```

```
              THE ESTIMATED PHYSICAL PROPERTIESOF

                             ACETONE

        T= 373.00 DEG K      P=    1.00 ATM      MOLE WT= 58.08

        373.00      DEG K,                T

          1.00      ATM,                  P

      30163.31      CC/G MOLE,            V

          0.986                           Z

        327.32      DEG K,                NORMAL BOILING PT.

         69.61      CC/G MOLE,            VOLUME AT NORMAL BOILING
                                                POINT

        515.73      DEG K,                TC

         58.78      ATM,                  PC

        189.87      CC/G MOLE,            VC

          0.264                           ZC

          4.057     ATM,                  VAPOR PRESSURE

          7.29                            RIEDEL FACTOR

          0.303                           ACENTRIC FACTOR

         21.657     CAL/G MOLE-DEG K,     CPO

         21.730     CAL/G MOLE-DEG K,     CP

         19.641     CAL/G MOLE-DEG K,     CV

          1.440     DEBYES,               DIPOLE MOMENT

        462.61      DEG K,                E/K

          4.504     ANGSTROMS,            INTERMOLECULAR DISTANCE

        115.26      CC/G MOLE,            HARD-SPHERE VOLUME

          0.01056   CENTIPOISE,           VISCOSITY AT LOW PRESSURE

          0.01088   CENTIPOISE,           VISCOSITY AT ELEVATED
                                                PRESSURE

          0.0000503 CAL/CM-SEC-DEG K,     THERMAL CONDUCTIVITY AT
                                                LOW PRESSURE
```

```
     METHOD FOR K NOT APPLICABLE

            29.11         CAL/G MOLE,          H(IDEAL)-H(IDEAL)-H(REAL)

             0.050        CAL/G MOLE-DEG K,  S(IDEAL)-S(REAL)

             1.015                             FUGACITY COEFFICIENT

          7346.1          CAL/G MOLE,          HEAT OF VAPORIZATION
                                                   AT NORMAL BOILING PT.

            22.443        CAL/G MOLE-DEG K,  ENTROPY OF VAPORIZATION
                                                   AT NORMAL BOILING PT.

           -52.634        KCAL/G MOLE,         HEAT OF FORMATION AT
                                                   STATED TEMPERATURE

           -51.840        KCAL/G MOLE,         HEAT OF FORMATION FOR
                                                   IDEAL GAS AT 1 ATM
                                                   AND 298 DEG K

           -59.918        CAL/G MOLE-DEG K,  ENTROPY OF FORMATION FOR
                                                   IDEAL GAS AT 1 ATM
                                                   AND 298 DEG K.

           -29.491        KCAL/G MOLE,         FREE ENERGY OF FORMATION
                                                   FOR IDEAL GAS AT 1
                                                   ATM AND 298 DEG K.
```

```
LIQUID PHYSICAL PROPERTIES

T=293.000000 DEG-K       P=  1.000000 ATM

      0.8642       GRAMS/CC              LIQUID DENSITY

SATURATED LIQUID ENTHALPY CALC
-3302.2976         CAL/G MOLE            LIQ. ENTHALPY DEPARTURE

REDUCED DENSITY>2.0 FOR BWR METHOD
REDUCED TEMPERATURE<0.6 FOR BWR METHOD
      2.7178       CAL/G MOLE-C          HT CAPACITY DEPARTURE

      0.3325       CENTIPOISE            LIQ VISCOSITY

    137.2000       (DYNES/CM)**1/4(CC/G MOLE)   PARACHOR

   -525.4514       CAL/G MOLE-K          LIQ ENTROPY DEPARTURE

    17.314987      DYNES/CM              SURFACE TENSION

     0.001349      1/DEG K               COEFF OF THRMAL EXP
```

```
                    THE ESTIMATED PHYSICAL PROPERTIESOF

                              ACETONITRILE

          T= 373.00 DEG K      P=    1.00 ATM      MOLE WT= 41.05

          373.00      DEG K,                 T

            1.00      ATM,                   P

        29987.71      CC/G MOLE,             V

            0.980                            Z

          345.43      DEG K,                 NORMAL BOILING PT.

           42.00      CC/G MOLE,             VOLUME AT NORMAL BOILING
                                                     POINT

          539.31      DEG K,                 TC

           47.77      ATM,                   PC

          244.06      CC/G MOLE,             VC

            0.263                            ZC

            2.268     ATM,                   VAPOR PRESSURE

            7.14                             RIEDEL FACTOR

            0.271                            ACENTRIC FACTOR

           14.202     CAL/G MOLE-DEG K,  CPO

           14.302     CAL/G MOLE-DEG K,  CP

           12.172     CAL/G MOLE-DEG K,  CV

            1.440     DEBYES,                DIPOLE MOMENT

          483.76      DEG K,                 E/K

            4.897     ANGSTROMS,             INTERMOLECULAR DISTANCE

          148.12      CC/G MOLE,             HARD-SPHERE VOLUME

            0.00753   CENTIPOISE,            VISCOSITY AT LOW PRESSURE

            0.00756   CENTIPOISE,            VISCOSITY AT ELEVATED
                                                     PRESSURE

            0.0000335 CAL/CM-SEC-DEG K,  THERMAL CONDUCTIVITY AT
                                                     LOW PRESSURE
```

```
     METHOD FOR K NOT APPLICABLE

            40.44        CAL/G MOLE,         H(IDEAL)-H(IDEAL)-H(REAL)

             0.069       CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

             1.021                           FUGACITY COEFFICIENT

          7388.4         CAL/G MOLE,         HEAT OF VAPORIZATION
                                                 AT NORMAL BOILING PT.

            21.386       CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                                 AT NORMAL BOILING PT.

            18.946       KCAL/G MOLE,        HEAT OF FORMATION AT
                                                 STATED TEMPERATURE

            19.380       KCAL/G MOLE,        HEAT OF FORMATION FOR
                                                 IDEAL GAS AT 1 ATM
                                                 AND 298 DEG K

            -4.422       CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                                 IDEAL GAS AT 1 ATM
                                                 AND 298 DEG K.

            21.029       KCAL/G MOLE,        FREE ENERGY OF FORMATION
                                                 FOR IDEAL GAS AT 1
                                                 ATM AND 298 DEG K.
```

```
   LIQUID PHYSICAL PROPERTIES

  T=293.000000 DEG-K      P=  1.000000 ATM

      0.4844       GRAMS/CC           LIQUID DENSITY

  SATURATED LIQUID ENTHALPY CALC
  -3447.2935       CAL/G MOLE         LIQ. ENTHALPY DEPARTURE

  REDUCED DENSITY>2.0 FOR BWR METHOD
  REDUCED TEMPERATURE<0.6 FOR BWR METHOD
      3.3376       CAL/G MOLE-C       HT CAPACITY DEPARTURE

  VISCOSITY CANNOT BE CALCULATED-NO INPUT DATA
     30.6000       (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

   -262.9148       CAL/G MOLE-K       LIQ ENTROPY DEPARTURE

    0.016959       DYNES/CM           SURFACE TENSION

    0.001265       1/DEG K            COEFF OF THRMAL EXP
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```
                    THE ESTIMATED PHYSICAL PROPERTIESOF

                                1-BUTENE

          T= 373.00 DEG K       P=    1.00 ATM     MOLE WT= 56.10

          373.00        DEG K,             T

            1.00        ATM,               P

        30229.34        CC/G MOLE,         V

            0.988                          Z

          268.90        DEG K,             NORMAL BOILING PT.

           89.04        CC/G MOLE,         VOLUME AT NORMAL BOILING
                                                POINT

          421.99        DEG K,             TC

           39.62        ATM,               PC

          236.44        CC/G MOLE,         VC

            0.270                          ZC

           16.696       ATM,               VAPOR PRESSURE

            6.77                           RIEDEL FACTOR

            0.195                          ACENTRIC FACTOR

           25.030       CAL/G MOLE-DEG K,  CPO

           25.096       CAL/G MOLE-DEG K,  CP

           23.018       CAL/G MOLE-DEG K,  CV

          248.90        DEG K,             E/K

            5.546       ANGSTROMS,         INTERMOLECULAR DISTANCE

          215.65        CC/G MOLE,         HARD-SPHERE VOLUME

            0.00989     CENTIPOISE,        VISCOSITY AT LOW PRESSURE

            0.01022     CENTIPOISE,        VISCOSITY AT ELEVATED
                                                PRESSURE

            0.0000593   CAL/CM-SEC-DEG K,  THERMAL CONDUCTIVITY AT
                                                LOW PRESSURE
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               0.0000590  CAL/CM-SEC-DEG K, THERMAL CONDUCTIVITY AT
                                                 ELEVATED PRESSURE

              25.60       CAL/G MOLE,       H(IDEAL)-H(IDEAL)-H(REAL)

               0.044      CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

               1.013                        FUGACITY COEFFICIENT

            5322.7        CAL/G MOLE,       HEAT OF VAPORIZATION
                                                 AT NORMAL BOILING PT.

              19.794      CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                                 AT NORMAL BOILING PT.

              -1.088      KCAL/G MOLE,      HEAT OF FORMATION AT
                                                 STATED TEMPERATURE

              -0.046      KCAL/G MOLE,      HEAT OF FORMATION FOR
                                                 IDEAL GAS AT 1 ATM
                                                 AND 298 DEG K

             -61.888      CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                                 IDEAL GAS AT 1 ATM
                                                 AND 298 DEG K.

              23.038      KCAL/G MOLE,      FREE ENERGY OF FORMATION
                                                 FOR IDEAL GAS AT 1
                                                 ATM AND 298 DEG K.
```

```
   LIQUID PHYSICAL PROPERTIES

  T=253.000000 DEG-K        P=  1.000000 ATM

      0.6448       GRAMS/CC               LIQUID DENSITY

  SATURATED LIQUID ENTHALPY CALC
  -2691.9548       CAL/G MOLE             LIQ. ENTHALPY DEPARTURE

  REDUCED DENSITY>2.0 FOR BWR METHOD
  REDUCED TEMPERATURE<0.6 FOR BWR METHOD
      1.4342       CAL/G MOLE-C           HT CAPACITY DEPARTURE

  VISCOSITY CANNOT BE CALCULATED-NO INPUT DATA
    160.0000       (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

   -312.0288       CAL/G MOLE-K           LIQ ENTROPY DEPARTURE

   11.348788       DYNES/CM               SURFACE TENSION

    0.001610       1/DEG K                COEFF OF THRMAL EXP
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```
                THE ESTIMATED PHYSICAL PROPERTIESOF

                          CHLOROBENZENE

       T= 423.00 DEG K       P=    1.00 ATM       MOLE WT=112.56

       423.00        DEG K,               T

         1.00        ATM,                 P

     33657.18        CC/G MOLE,           V

         0.970                            Z

       445.26        DEG K,               NORMAL BOILING PT.

       117.57        CC/G MOLE,           VOLUME AT NORMAL BOILING
                                                  POINT

       692.35        DEG K,               TC

        44.86        ATM,                 PC

       314.88        CC/G MOLE,           VC

         0.249                            ZC

         0.553       ATM,                 VAPOR PRESSURE

         7.11                             RIEDEL FACTOR

         0.265                            ACENTRIC FACTOR

        30.376       CAL/G MOLE-DEG K,    CPO

        30.522       CAL/G MOLE-DEG K,    CP

        28.321       CAL/G MOLE-DEG K,    CV

         1.440       DEBYES,              DIPOLE MOMENT

       621.04        DEG K,               E/K

         5.330       ANGSTRUMS,           INTERMOLECULAR DISTANCE

       191.04        CC/G MOLE,           HARD-SPHERE VOLUME

         0.01050     CENTIPOISE,          VISCOSITY AT LOW PRESSURE

         0.01054     CENTIPOISE,          VISCOSITY AT ELEVATED
                                                  PRESSURE

         0.0000337   CAL/CM-SEC-DEG K,    THERMAL CONDUCTIVITY AT
                                                  LOW PRESSURE
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```
          METHOD FOR K NOT APPLICABLE

               67.84       CAL/G MOLE,        H(IDEAL)-H(IDEAL)-H(REAL)

               0.101       CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

               1.032                          FUGACITY COEFFICIENT

              9398.4       CAL/G MOLE,        HEAT OF VAPORIZATION
                                                  AT NORMAL BOILING PT.

              21.108       CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                                  AT NORMAL BOILING PT.

          HEAT OF FORMATION AT T= 423.00 CAN NOT BE CALC. DUE TO
              STIPULATIONS ON METHODS.
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```
LIQUID PHYSICAL PROPERTIES

T=293.000000 DEG=K      P=  1.000000 ATM

     1.1386      GRAMS/CC            LIQUID DENSITY

SATURATED LIQUID ENTHALPY CALC
=5383.8750      CAL/G MOLE          LIQ. ENTHALPY DEPARTURE

REDUCED DENSITY>2.0 FOR BWR METHOD
REDUCED TEMPERATURE<0.6 FOR BWR METHOD
     9.2276      CAL/G MOLE-C        HT CAPACITY DEPARTURE

     0.7609      CENTIPOISE          LIQ VISCOSITY

   186.0996      (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

   -15.8554      CAL/G MOLE-K        LIQ ENTROPY DEPARTURE

  12.555371      DYNES/CM            SURFACE TENSION

   0.000928      1/DEG K             COEFF OF THRMAL EXP
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                    THE ESTIMATED PHYSICAL PROPERTIESOF

                              CYCLOPENTANE

           T= 373.00 DEG K      P=    1.00 ATM      MOLE WT= 70.13

            373.00       DEG K,              T

              1.00       ATM,                P

          29672.72       CC/G MOLE,          V

              0.969                          Z

            381.95       DEG K,              NORMAL BOILING PT.

            116.47       CC/G MOLE,          VOLUME AT NORMAL BOILING
                                                     POINT

            608.43       DEG K,              TC

             44.17       ATM,                PC

            311.60       CC/G MOLE,          VC

              0.276                          ZC

              0.775      ATM,                VAPOR PRESSURE

              6.69                           RIEDEL FACTOR

              0.161                          ACENTRIC FACTOR

             27.486      CAL/G MOLE-DEG K,   CPO

             27.633      CAL/G MOLE-DEG K,   CP

             25.430      CAL/G MOLE-DEG K,   CV

            384.32       DEG K,              E/K

              5.943      ANGSTROMS,          INTERMOLECULAR DISTANCE

            265.37       CC/G MOLE,          HARD-SPHERE VOLUME

              0.00844    CENTIPOISE,         VISCOSITY AT LOW PRESSURE

              0.00682    CENTIPOISE,         VISCOSITY AT ELEVATED
                                                     PRESSURE

              0.0000393  CAL/CM-SEC-DEG K,   THERMAL CONDUCTIVITY AT
                                                     LOW PRESSURE
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      0.0000391  CAL/CM-SEC-DEG K, THERMAL CONDUCTIVITY AT
                                                ELEVATED PRESSURE

     60.23       CAL/G MOLE,       H(IDEAL)-H(IDEAL)-H(REAL)

      0.102      CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

      1.032                        FUGACITY COEFFICIENT

   7618.1        CAL/G MOLE,       HEAT OF VAPORIZATION
                                                AT NORMAL BOILING PT.

     19.945      CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                                AT NORMAL BOILING PT.

    -20.586      KCAL/G MOLE,      HEAT OF FORMATION AT
                                                STATED TEMPERATURE

    -18.950      KCAL/G MOLE,      HEAT OF FORMATION FOR
                                                IDEAL GAS AT 1 ATM
                                                AND 298 DEG K

    -92.160      CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                                IDEAL GAS AT 1 ATM
                                                AND 298 DEG K.

     15.426      KCAL/G MOLE,      FREE ENERGY OF FORMATION
                                                FOR IDEAL GAS AT 1
                                                ATM AND 298 DEG K.
```

```
   LIQUID PHYSICAL PROPERTIES


  T=293.000000 DEG-K       P=  1.000000 ATM

      0.6476       GRAMS/CC             LIQUID DENSITY

  SATURATED LIQUID ENTHALPY CALC
  -3886.0454       CAL/G MOLE           LIQ. ENTHALPY DEPARTURE

  REDUCED DENSITY>2.0 FOR BWR METHOD
  REDUCED TEMPERATURE<0.6 FOR BWR METHOD
      5.2396       CAL/G MOLE-C         HT CAPACITY DEPARTURE

  VISCOSITY CANNOT BE CALCULATED-NO INPUT DATA
    200.0000       (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

   -226.1269       CAL/G MOLE-K         LIQ ENTROPY DEPARTURE

   11.623533       DYNES/CM             SURFACE TENSION

    0.001079       1/DEG K              COEFF OF TH-MAL EXP
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          THE ESTIMATED PHYSICAL PROPERTIESOF

                     ETHANE

  T= 373.00 DEG K     P=    1.00 ATM     MOLE WT= 30.07

  373.00       DEG K,            T

    1.00       ATM,              P

30478.73       CC/G MOLE,        V

    0.996                        Z

  188.32       DEG K,            NORMAL BOILING PT.

   56.47       CC/G MOLE,        VOLUME AT NORMAL BOILING
                                      POINT

  311.06       DEG K,            TC

   47.70       ATM,              PC

  151.87       CC/G MOLE,        VC

    0.284                        ZC

  158.972      ATM,              VAPOR PRESSURE

    6.29                         RIEDEL FACTOR

    0.099                        ACENTRIC FACTOR

   14.953      CAL/G MOLE-DEG K, CPG

   14.979      CAL/G MOLE-DEG K, CP

   12.958      CAL/G MOLE-DEG K, CV

  218.07       DEG K,            E/K

    4.518      ANGSTROMS,        INTERMOLECULAR DISTANCE

  116.54       CC/G MOLE,        HARD-SPHERE VOLUME

    0.01132    CENTIPOISE,       VISCOSITY AT LOW PRESSURE

    0.01134    CENTIPOISE,       VISCOSITY AT ELEVATED
                                      PRESSURE

    0.0000742  CAL/CM-SEC-DEG K, THERMAL CONDUCTIVITY AT
                                      LOW PRESSURE
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    0.0000740  CAL/CM-SEC-DEG K, THERMAL CONDUCTIVITY AT
                                      ELEVATED PRESSURE

    9.39       CAL/G MOLE,       H(IDEAL)-H(IDEAL)-H(REAL)

    0.017      CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

    1.004                        FUGACITY COEFFICIENT

 3589.8        CAL/G MOLE,       HEAT OF VAPORIZATION
                                      AT NORMAL BOILING PT.

   19.063      CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                      AT NORMAL BOILING PT.

  -21.108      KCAL/G MOLE,      HEAT OF FORMATION AT
                                      STATED TEMPERATURE

  -20.240      KCAL/G MOLE,      HEAT OF FORMATION FOR
                                      IDEAL GAS AT 1 ATM
                                      AND 298 DEG K

  -41.455      CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                      IDEAL GAS AT 1 ATM
                                      AND 298 DEG K.

   -4.777      KCAL/G MOLE,      FREE ENERGY OF FORMATION
                                      FOR IDEAL GAS AT 1
                                      ATM AND 298 DEG K.
```

```
LIQUID PHYSICAL PROPERTIES


T=180.000000 DEG-K       P= 1.000000 ATM

   0.5267       GRAMS/CC              LIQUID DENSITY

SATURATED LIQUID ENTHALPY CALC
-3297.4539      CAL/G MOLE            LIQ. ENTHALPY DEPARTURE

REDUCED DENSITY>2.0 FOR BWR METHOD
REDUCED TEMPERATURE<0.6 FOR BWR METHOD
   2.3540       CAL/G MOLE-C          HT CAPACITY DEPARTURE

VISCOSITY CANNOT BE CALCULATED-NO INPUT DATA
  110.4000      (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

 -600.5671      CAL/G MOLE-K          LIQ ENTROPY DEPARTURE

 13.862657      DYNES/CM              SURFACE TENSION

  0.001895      1/DEG K               COEFF OF THRMAL EXP
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                    THE ESTIMATED PHYSICAL PROPERTIESOF

                                ETHYL ALCOHOL

         T= 373.00 DEG K      P=   1.00 ATM      MOLE WT= 46.07

         373.00        DEG K,                 T

           1.00        ATM,                   P

       30197.65        CC/G MOLE,             V

          0.987                               Z

         346.68        DEG K,                 NORMAL BOILING PT.

          61.16        CC/G MOLE,             VOLUME AT NORMAL BOILING
                                                      POINT

         514.28        DEG K,                 TC

          63.17        ATM,                   PC

         167.63        CC/G MOLE,             VC

          0.251                               ZC

          2.571        ATM,                   VAPOR PRESSURE

           8.68                               RIEDEL FACTOR

          0.584                               ACENTRIC FACTOR

         18.719        CAL/G MOLE-DEG K,      CPO

         18.787        CAL/G MOLE-DEG K,      CP

         16.706        CAL/G MOLE-DEG K,      CV

          1.440        DEBYES,                DIPOLE MOMENT

         429.39        DEG K,                 E/K

          4.534        ANGSTROMS,             INTERMOLECULAR DISTANCE

         117.57        CC/G MOLE,             HARD-SPHERE VOLUME

          0.00992      CENTIPOISE,            VISCOSITY AT LOW PRESSURE

          0.00994      CENTIPOISE,            VISCOSITY AT ELEVATED
                                                      PRESSURE

          0.0000521    CAL/CM-SEC-DEG K,      THERMAL CONDUCTIVITY AT
                                                      LOW PRESSURE
```

```
          METHOD FOR K NOT APPLICABLE

               26.86        CAL/G MOLE,           H(IDEAL)-H(IDEAL)-H(REAL)

               0.046        CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

               1.014                              FUGACITY COEFFICIENT

              9103.7        CAL/G MOLE,           HEAT OF VAPORIZATION
                                                      AT NORMAL BOILING PT.

               26.259       CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                                      AT NORMAL BOILING PT.

              -57.672       KCAL/G MOLE,          HEAT OF FORMATION AT
                                                      STATED TEMPERATURE

              -56.946       KCAL/G MOLE,          HEAT OF FORMATION FOR
                                                      IDEAL GAS AT 1 ATM
                                                      AND 298 DEG K

              -53.557       CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                                      IDEAL GAS AT 1 ATM
                                                      AND 298 DEG K.

              -36.969       KCAL/G MOLE,          FREE ENERGY OF FORMATION
                                                      FOR IDEAL GAS AT 1
                                                      ATM AND 298 DEG K.
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```
LIQUID PHYSICAL PROPERTIES

T=293.000000 DEG-K       P=  1.000000 ATM

     0.8006       GRAMS/CC            LIQUID DENSITY

SATURATED LIQUID ENTHALPY CALC
-4071.2495        CAL/G MOLE          LIQ. ENTHALPY DEPARTURE

REDUCED DENSITY>2.0 FOR BWR METHOD
REDUCED TEMPERATURE<0.6 FOR BWR METHOD
     2.3581       CAL/G MOLE-C        HT CAPACITY DEPARTURE

     1.2118       CENTIPOISE          LIQ VISCOSITY

   127.5999       (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

  -228.0041       CAL/G MOLE-K        LIQ ENTROPY DEPARTURE

  24.136931       DYNES/CM            SURFACE TENSION

   0.001354       1/DEG K             COEFF OF THERMAL EXP
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```
                    THE ESTIMATED PHYSICAL PROPERTIESOF

                                ETHYL AMINE

          T= 373.00 DEG K      P=    2.00 ATM      MOLE WT= 45.08

      373.00        DEG K,                     T

        2.00        ATM,                       P

    14959.90        CC/G MOLE,                 V

        0.978                                  Z

      293.46        DEG K,                     NORMAL BOILING PT.

       66.01        CC/G MOLE,                 VOLUME AT NORMAL BOILING
                                                    POINT

      463.63        DEG K,                     TC

       57.04        ATM,                       PC

      179.68        CC/G MOLE,                 VC

        0.269                                  ZC

       10.637       ATM,                       VAPOR PRESSURE

        7.20                                   RIEDEL FACTOR

        0.284                                  ACENTRIC FACTOR

       21.805       CAL/G MOLE-DEG K,          CPO

       21.862       CAL/G MOLE-DEG K,          CP

       19.711       CAL/G MOLE-DEG K,          CV

        1.440       DEBYES,                    DIPOLE MOMENT

      415.87        DEG K,                     E/K

        4.422       ANGSTROMS,                 INTERMOLECULAR DISTANCE

      109.08        CC/G MOLE,                 HARD-SPHERE VOLUME

        0.01050     CENTIPOISE,                VISCOSITY AT LOW PRESSURE

        0.01054     CENTIPOISE,                VISCOSITY AT ELEVATED
                                                    PRESSURE

        0.0000658   CAL/CM-SEC-DEG K,          THERMAL CONDUCTIVITY AT
                                                    LOW PRESSURE
```

```
    METHOD FOR K NOT APPLICABLE

          45.90      CAL/G MOLE,          H(IDEAL)-H(IDEAL)-H(REAL)

          0.079      CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

          1.023                           FUGACITY COEFFICIENT

         6486.8      CAL/G MOLE,          HEAT OF VAPORIZATION
                                             AT NORMAL BOILING PT.

         22.105      CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                             AT NORMAL BOILING PT.

        -12.898      KCAL/G MOLE,         HEAT OF FORMATION AT
                                             STATED TEMPERATURE

        -12.246      KCAL/G MOLE,         HEAT OF FORMATION FOR
                                             IDEAL GAS AT 1 ATM
                                             AND 298 DEG K

        -74.944      CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                             IDEAL GAS AT 1 ATM
                                             AND 298 DEG K.

         15.706      KCAL/G MOLE,         FREE ENERGY OF FORMATION
                                             FOR IDEAL GAS AT 1
                                             ATM AND 298 DEG K.
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```
            LIQUID PHYSICAL PROPERTIES

          T=280.000000 DEG-K       P=  1.000000 ATM

              0.6816       GRAMS/CC            LIQUID DENSITY

          SATURATED LIQUID ENTHALPY CALC
          -2968.0356       CAL/G MOLE          LIQ. ENTHALPY DEPARTURE

          REDUCED DENSITY>2.0 FOR BWR METHOD
              2.1068       CAL/G MOLE-C        HT CAPACITY DEPARTURE

          VISCOSITY CANNOT BE CALCULATED-NO INPUT DATA
            138.9998       (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

           -694.6428       CAL/G MOLE-K        LIQ ENTROPY DEPARTURE

           19.387833       DYNES/CM            SURFACE TENSION

            0.001526       1/DEG K             COEFF OF THERMAL EXP
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```
                    THE ESTIMATED PHYSICAL PROPERTIESOF

                              ETHYL BROMIDE

          T= 373.00 DEG K      P=    1.00 ATM      MOLE WT=108.98

           373.00        DEG K,              T

             1.00        ATM,                P

         30227.80        CC/G MOLE,          V

             0.988                           Z

           310.75        DEG K,              NORMAL BOILING PT.

            62.15        CC/G MOLE,          VOLUME AT NORMAL BOILING
                                                     POINT

           505.69        DEG K,              TC

            65.08        ATM,                PC

           170.69        CC/G MOLE,          VC

             0.268                           ZC

             6.261       ATM,                VAPOR PRESSURE

             6.91                            RIEDEL FACTOR

             0.239                           ACENTRIC FACTOR

            18.275       CAL/G MOLE-DEG K,   CPO

            18.358       CAL/G MOLE-DEG K,   CP

            16.264       CAL/G MOLE-DEG K,   CV

             1.440       DEBYES,             DIPOLE MOMENT

           453.60        DEG K,              E/K

             4.347       ANGSTROMS,          INTERMOLECULAR DISTANCE

           103.63        CC/G MOLE,          HARD-SPHERE VOLUME

             0.01612     CENTIPOISE,         VISCOSITY AT LOW PRESSURE

             0.01615     CENTIPOISE,         VISCOSITY AT ELEVATED
                                                     PRESSURE

             0.0000350   CAL/CM-SEC-DEG K,   THERMAL CONDUCTIVITY AT
                                                     LOW PRESSURE
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```
      METHOD FOR K NOT APPLICABLE

             24.93        CAL/G MOLE,          H(IDEAL)-H(IDEAL)-H(REAL)

              0.043       CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

              1.013                         FUGACITY COEFFICIENT

           6747.6         CAL/G MOLE,       HEAT OF VAPORIZATION
                                                   AT NORMAL BOILING PT.

             21.714       CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                                   AT NORMAL BOILING PT.

      HEAT OF FORMATION AT T= 373.00 CAN NOT BE CALC. DUE TO
           STIPULATIONS ON METHODS.
```

```
    LIQUID PHYSICAL PROPERTIES

    T=293.000000 DEG-K        P=  1.000000 ATM

         1.7691        GRAMS/CC               LIQUID DENSITY

    SATURATED LIQUID ENTHALPY CALC
    -3240.2122         CAL/G MOLE             LIQ. ENTHALPY DEPARTURE

    REDUCED DENSITY>2.0 FOR BWR METHOD
    REDUCED TEMPERATURE<0.6 FOR BWR METHOD
         2.6265        CAL/G MOLE-C           HT CAPACITY DEPARTURE

         0.3988        CENTIPOISE             LIQ VISCOSITY

       161.7998        (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

      -801.8662        CAL/G MOLE-K           LIQ ENTROPY DEPARTURE

      47.358276        DYNES/CM               SURFACE TENSION

       0.001389        1/DEG K                COEFF OF THRMAL EXP
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                THE ESTIMATED PHYSICAL PROPERTIESOF

                         ETHYLACETYLENE

        T= 298.00 DEG K      P=    1.00 ATM      MOLE WT= 54.09

        298.00       DEG K,               T

          1.00       ATM,                 P

      24086.74       CC/G MOLE,           V

         0.985                            Z

        231.76       DEG K,               NORMAL BOILING PT.

         78.11       CC/G MOLE,           VOLUME AT NORMAL BOILING
                                                POINT

        377.15       DEG K,               TC

         44.70       ATM,                 PC

        209.14       CC/G MOLE,           VC

         0.302                            ZC

         3.900       ATM,                 VAPOR PRESSURE

          6.40                            RIEDEL FACTOR

         0.122                            ACENTRIC FACTOR

        21.388       CAL/G MOLE-DEG K,    CPO

        21.464       CAL/G MOLE-DEG K,    CP

        19.370       CAL/G MOLE-DEG K,    CV

        331.11       DEG K,               E/K

         4.663       ANGSTROMS,           INTERMOLECULAR DISTANCE

        128.16       CC/G MOLE,           HARD-SPHERE VOLUME

         0.01049     CENTIPOISE,          VISCOSITY AT LOW PRESSURE

         0.01085     CENTIPOISE,          VISCOSITY AT ELEVATED
                                                PRESSURE

         0.0000556   CAL/CM-SEC-DEG K,    THERMAL CONDUCTIVITY AT
                                                LOW PRESSURE
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      0.0000554  CAL/CM-SEC-DEG K, THERMAL CONDUCTIVITY AT
                                            ELEVATED PRESSURE

     24.34       CAL/G MOLE,       H(IDEAL)-H(IDEAL)-H(REAL)

      0.052      CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

      1.015                        FUGACITY COEFFICIENT

   4445.6        CAL/G MOLE,       HEAT OF VAPORIZATION
                                            AT NORMAL BOILING PT.

     19.182      CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                            AT NORMAL BOILING PT.

     39.394      KCAL/G MOLE,      HEAT OF FORMATION AT
                                            STATED TEMPERATURE

     39.394      KCAL/G MOLE,      HEAT OF FORMATION FOR
                                            IDEAL GAS AT 1 ATM
                                            AND 298 DEG K

    -35.377      CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                            IDEAL GAS AT 1 ATM
                                            AND 298 DEG K.

     49.936      KCAL/G MOLE,      FREE ENERGY OF FORMATION
                                            FOR IDEAL GAS AT 1
                                            ATM AND 298 DEG K.
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        LIQUID PHYSICAL PROPERTIES

       T=200.000000 DEG-K       P=  1.000000 ATM

          0.6744      GRAMS/CC            LIQUID DENSITY

       SATURATED LIQUID ENTHALPY CALC
       -3950.8936     CAL/G MOLE          LIQ. ENTHALPY DEPARTURE

       REDUCED DENSITY>2.0 FOR BWR METHOD
       REDUCED TEMPERATURE<0.6 FOR BWR METHOD
          3.5654      CAL/G MOLE-C        HT CAPACITY DEPARTURE

       VISCOSITY CANNOT BE CALCULATED-NO INPUT DATA
        129.5999      (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

        -498.4290     CAL/G MOLE-K        LIQ ENTROPY DEPARTURE

        6.794670      DYNES/CM            SURFACE TENSION

        0.001562      1/DEG K             COEFF OF THRMAL EXP



TRAN ** STOP

00:01:10
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                 THE ESTIMATED PHYSICAL PROPERTIESOF

                                METHANE

          T= 373.00 DEG K      P=    1.00 ATM      MOLE WT= 16.04

          373.00       DEG K,              T

            1.00       ATM,                P

        30536.13       CC/G MOLE,          V

            0.998                          Z

          153.43       DEG K,              NORMAL BOILING PT.

           35.00       CC/G MOLE,          VOLUME AT NORMAL BOILING
                                                   POINT

          261.56       DEG K,              TC

           49.89       ATM,                PC

          124.06       CC/G MOLE,          VC

            0.288                          ZC

          567.809      ATM,                VAPOR PRESSURE

            5.97                           RIEDEL FACTOR

            0.032                          ACENTRIC FACTOR

            7.477      CAL/G MOLE-DEG K,   CPO

            7.492      CAL/G MOLE-DEG K,   CP

            5.484      CAL/G MOLE-DEG K,   CV

          194.30       DEG K,              E/K

            4.143      ANGSTROMS,          INTERMOLECULAR DISTANCE

           89.85       CC/G MOLE,          HARD-SPHERE VOLUME

            0.01015    CENTIPOISE,         VISCOSITY AT LOW PRESSURE

            0.01016    CENTIPOISE,         VISCOSITY AT ELEVATED
                                                   PRESSURE

            0.0000636  CAL/CM-SEC-DEG K,   THERMAL CONDUCTIVITY AT
                                                   LOW PRESSURE
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     0.0000634  CAL/CM-SEC-DEG K, THERMAL CONDUCTIVITY AT
                                           ELEVATED PRESSURE

     5.58       CAL/G MOLE,       H(IDEAL)-H(IDEAL)-H(REAL)

     0.011      CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

     1.002                        FUGACITY COEFFICIENT

  2802.6        CAL/G MOLE,       HEAT OF VAPORIZATION
                                           AT NORMAL BOILING PT.

    18.266      CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                           AT NORMAL BOILING PT.

   -10.554      KCAL/G MOLE,      HEAT OF FORMATION AT
                                           STATED TEMPERATURE

   -10.120      KCAL/G MOLE,      HEAT OF FORMATION FOR
                                           IDEAL GAS AT 1 ATM
                                           AND 298 DEG K

   -19.263      CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                           IDEAL GAS AT 1 ATM
                                           AND 298 DEG K.

    -2.927      KCAL/G MOLE,      FREE ENERGY OF FORMATION
                                           FOR IDEAL GAS AT 1
                                           ATM AND 298 DEG K.
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      LIQUID PHYSICAL PROPERTIES

     T=100.000000 DEG-K       P=  1.000000 ATM

         0.3763        GRAMS/CC             LIQUID DENSITY

     SATURATED LIQUID ENTHALPY CALC
     -2795.3079        CAL/G MOLE           LIQ. ENTHALPY DEPARTURE

     REDUCED DENSITY>2.0 FOR BWR METHOD
     REDUCED TEMPERATURE<0.6 FOR BWR METHOD
        13.3670        CAL/G MOLE-C         HT CAPACITY DEPARTURE

     VISCOSITY CANNOT BE CALCULATED-NO INPUT DATA
        70.4000        (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

      -147.3971        CAL/G MOLE-K         LIQ ENTROPY DEPARTURE

       7.437118        DYNES/CM             SURFACE TENSION

       0.001657        1/DEG K              COEFF OF THRMAL EXP
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              THE ESTIMATED PHYSICAL PROPERTIESOF

                              PHENOL

        T= 473.00 DEG K      P=    1.00 ATM      MOLE WT= 94.11

       473.00      DEG K,                 T

         1.00      ATM,                   P

     38162.00      CC/G MOLE,             V

         0.984                            Z

       454.11      DEG K,                 NORMAL BOILING PT.

        79.98      CC/G MOLE,             VOLUME AT NORMAL BOILING
                                                POINT

       690.35      DEG K,                 TC

        60.81      ATM,                   PC

       218.64      CC/G MOLE,             VC

         0.235                            ZC

         1.659     ATM,                   VAPOR PRESSURE

         8.04                             RIEDEL FACTOR

         0.454                            ACENTRIC FACTOR

        35.061     CAL/G MOLE-DEG K,  CPO

        35.161     CAL/G MOLE-DEG K,  CP

        33.061     CAL/G MOLE-DEG K,  CV

         1.440     DEBYES,                DIPOLE MOMENT

       752.81      DEG K,                 E/K

         4.123     ANGSTROMS,             INTERMOLECULAR DISTANCE

        88.40      CC/G MOLE,             HARD-SPHERE VOLUME

         0.01626   CENTIPOISE,            VISCOSITY AT LOW PRESSURE

         0.01628   CENTIPOISE,            VISCOSITY AT ELEVATED
                                                PRESSURE

         0.0000727 CAL/CM-SEC-DEG K,  THERMAL CONDUCTIVITY AT
                                                LOW PRESSURE
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          METHOD FOR K NOT APPLICABLE

              41.09     CAL/G MOLE,           H(IDEAL)-H(IDEAL)-H(REAL)

              0.055     CAL/G MOLE-DEG K, S(IDEAL)-S(REAL)

              1.017                           FUGACITY COEFFICIENT

            11132.6     CAL/G MOLE,           HEAT OF VAPORIZATION
                                                  AT NORMAL BOILING PT.

             24.515     CAL/G MOLE-DEG K, ENTROPY OF VAPORIZATION
                                                  AT NORMAL BOILING PT.

            -25.551     KCAL/G MOLE,          HEAT OF FORMATION AT
                                                  STATED TEMPERATURE

            -24.830     KCAL/G MOLE,          HEAT OF FORMATION FOR
                                                  IDEAL GAS AT 1 ATM
                                                  AND 298 DEG K

            -47.301     CAL/G MOLE-DEG K, ENTROPY OF FORMATION FOR
                                                  IDEAL GAS AT 1 ATM
                                                  AND 298 DEG K.

             -2.457     KCAL/G MOLE,          FREE ENERGY OF FORMATION
                                                  FOR IDEAL GAS AT 1
                                                  ATM AND 298 DEG K.


ORTRAN ** STOP

T  00:00:26
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    LIQUID PHYSICAL PROPERTIES

    T=293.000000 DEG-K       P=  1.000000 ATM

         1.3880       GRAMS/CC               LIQUID DENSITY

    SATURATED LIQUID ENTHALPY CALC
    -5581.3750        CAL/G MOLE             LIQ. ENTHALPY DEPARTURE

    REDUCED DENSITY>2.0 FOR BWR METHOD
    REDUCED TEMPERATURE<0.6 FOR BWR METHOD
         9.2563       CAL/G MOLE-C          HT CAPACITY DEPARTURE

         4.3669       CENTIPOISE             LIQ VISCOSITY

       165.9998       (DYNES/CM)**1/4(CC/G MOLE)  PARACHOR

       108.3379       CAL/G MOLE-K           LIQ ENTROPY DEPARTURE

      35.922058       DYNES/CM               SURFACE TENSION

       0.000931       1/DEG K                COEFF OF THERMAL EXP
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