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SUBJECT: UCRL-19011, "COMPUTER PROGRAMS FOR AN IMPROVED EQUATION OF STATE
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Please add the corrected pages: 52a, 52b, and 52c to subject report. Replace corrected pages: 53, 54, 55, 56, 57, 58 and 59 with the attached sheets.

COMPUTER PROGRAMS FOR AN IMPROVED EQUATION OF STATE
(ES68Z AND ES68M)

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May 1969

Abstract

Two Fortran programs for the use of the new modification of the equation of state of Redlich and Kwong are presented and their application is described in detail. Program ES68Z computes compressibility factor for a flexible temperature-pressure schedule. Program ES68M leads, in addition, to fugacity coefficients, enthalpies and entropies. It can be used for mixtures and furnishes individual fugacity coefficients.

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The improved equation of state described in UCRL-19010 requires automatic computation. Two separate programs have been developed.

ES68Z is able to compute experimental compressibility factors from PVT-data of any kind; in addition, it allows for a very flexible T-P schedule. But it is restricted to pure substances (or mixtures of fixed composition with prescribed parameters) and it computes only compressibility factors.

ES68M computes compressibility factors, fugacity coefficients, computes parameter combinations and also individual fugacity coefficients for mixtures, and computes enthalpy and entropy. It is restricted to equidistant pressure values on arbitrarily selected isothermals.

1. The Program ES68Z
11. General Scope

The program ES68Z - Equation of State 1968 - can be used for the computation of the compressibility factor $Z = PV/RT$ for pure substances. It is based on a modification of the equation of state by Redlich and Kwong, containing a third individual parameter.

The program ES68Z is written in Fortran IV. It consists of the main program ES68Z and the subroutine VIETA.

The main program ES68Z can be divided into four major parts: (1) Input and Preparation, (2) Main Cycle, (3) Approximation Cycle, and (4) Results.

The data cards to be introduced are: (1) the Title Card which states the title of the problem. The integer KCL controls intermediate quantities to be printed out. MCL is used to indicate the kind of experimental data to be read in. The experimental data may be given as compressibility factors Z; if PV, volume or density are given, the program converts the data to Z. WOM (molar weight of the substance) is to be punched on the Title Card when the observed data are expressed in mass or volume units instead of molar units. (2) Experimental Data are given as Z, or PV, volume or density. A blank card follows the last data card. (3) the Substance Card gives the name of the substance, the critical temperature (TC), pressure (PC) and compressibility factor (ZC). The last quantity LAA controls the number of approximation cycles desired. (4) the Temperature-Pressure Schedule Cards allow a variety of prescriptions for different sets of temperatures and pressures. The T-schedule provides for sets consisting of a starting temperature TL and an arbitrary

number of higher temperatures $TL + DT$, $TL + 2DT$, $TL + 3DT$, at equal intervals. The P-schedule may follow one of the three schemes: (a) starting pressure PL and any number of higher pressures $PL + DP$, $PL + 2DP$, $PL + 3DP$, at equal intervals, (b) starting pressure PL and any number of pressures of the amounts $2PL$, $5PL$, $10PL$, etc., (c) starting pressure PL plus any number of additional pressures read in on cards following the Schedule Card. Several sets of T-P schedules may be put in provided the total number of points (product of NOT and NOP) does not exceed 500. Any positive value for KS in the schedule card means that another schedule card follows. The last schedule card carries $KS = 0$. Calculation for a new substance can be prescribed simply by adding a new complete set starting with the Title Card and so on. A card containing $KCL = -1$ will terminate the computation.

The data are to be given in arbitrary but consistent absolute units throughout, e.g., all temperatures in $^{\circ}K$ or $^{\circ}R$, and pressures in atm, psia, etc. The output is given in the same units.

The program can also be used for computations starting from the reduced variables T_r and P_r . In this case, both T_c and P_c are set at 1 and T_r and P_r are introduced wherever T and P are prescribed.

The subroutine used in this program is VIETA-MODIFICATION 4 to solve the general cubic equation. This is a modified version of a SHARE routine. The solution gives any of the three cases: two equal roots ($MTYPE=0$), two complex roots ($MTYPE=1$) and three real roots ($MTYPE=-1$).

12. Outline of the Program

The first part (addresses 101 to 199) takes care of the input and assigns a point number ME to every experimental value ZE and the corresponding values of T_r and P_r as prescribed in the T-P schedule.

In the Main Cycle (addresses 201 to 299) the computation of ZE is carried out if ZE is given by data for density, volume or PV. The results of the equation of Redlich and Kwong and several coefficients of the modified cubic equation are computed.

In the Approximation Cycle (addresses 301 to 399) the coefficients A(2), A(3), A(4) of the modified cubic equation are computed. The subroutine VIETA furnishes the first results, which are fed-back. The final result is mixed with the result of Redlich and Kwong if $T_r > 1$. In this case also the deviation function DC is computed and added.

The last part (addresses 401 to 499) takes care of the main output and of the return to a new problem.

In the following the symbols used in the text and in the program are coordinated.

Symbols in Program	Symbols in Text
AC	A
AK	A_k
BC	B
BK	B_k
D	V_c/V
DC	Z_D
GG	G
GL	L
PA	P
PRR	P_r
QZ	c_{12}
TK	T

TRR	T_r
TT	T_r^3
U	c_5
UF	c_{10}
UG	c_{11}
V	c_4
VF	c_8
VG	c_8
W	c_1
WA	c_2
WB	c_3
WF	c_6
WG	c_7
ZF	Z
ZFK	Z_K
ZG	Z
ZGG	Z_M

13. Input

1. Title Card

Column

- 2-37 Title of the problem.
- 38-39 KCL = Print intermediate quantities: 0 no print
9 print
-1 termination
- 40-41 MCL: Experimental data
If MCL = 0: no data;
MCL > 0: data.

If MCL = 1, data are given as Z, but
if MCL > 1, data are given as PV,
or volume, or density.

- 42-43 NPC: Reserved for punch control (not included in the program).
- 44-53(4 dec.) WOM: molar weight (if required for the computation of experimental Z).
- 54-63(4 dec.) ECL: not used in this program.

The following list shows the values of MCL and WOM to be used when the set of experimental data is given as PV, or volume or density; WOM = 0 when the data are given as Z.

	<u>Units</u>		<u>MCL</u>	<u>WOM</u>
for P	for T	for volume or density		
atm	°K	amagat	2	0
atm	°K	cm ³ /g	23	MW
atm	°K	g/cm ³	21	MW
atm	°K	lit/mole	23	0
atm	°K	moles/lit	21	0
mmHg	°K	lit/mole	3	0
psia	°R	cu ft/lb	33	MW
psia	°R	lb/cu ft	31	MW
psia	°R	cu ft/lb-mole	33	0
psia	°R	lb-mole/cu ft	31	0

2. Experimental Data (only if MCL ≥ 1)

Insert any number of cards up to 499.

Column

- 2-10(4 dec.) ZE: Experimental value of Z or PV or volume or density. No card with ZE = 0 is allowed.

The last card is followed by a blank card.

3. Substance Card

Column

2-24	Name of the substance.
25-36(6 dec.)	TC: critical temperature in any absolute units.
37-48(6 dec.)	PC: critical pressure in any absolute units.
49-60(6 dec.)	ZC: critical compressibility factor.
61-62	LAA: number of approximation cycles; if LAA = 0, computer sets LAA = 40 if LAA > 0, computer sets number of approximation cycles LA = LAA + 10.

4. T-P Schedule Cards

Column

3-4	KS: control KS > 0 indicates that the schedule card is to be followed by another one, while KS = 0 means that the schedule card is the last in the set.
5-6	NOT: number of temperatures to be introduced.
7-8	NOP: number of pressures to be introduced.
9-20(6 dec.)	TL: lowest temperature to be introduced, in the same unit as TC.
21-32(6 dec.)	DT: temperature increment in the same unit as TC.
33-44(6 dec.)	PL: lowest pressure to be introduced, in the same unit as PC.
45-56(6 dec.)	DP = -1: pressure schedule is PL, 2PL, 5PL, 10 PL, etc. for NOP pressures. DP = 0: schedule is given by PL and the following NOP-1 additional pressure cards. DP > 0: pressure increment for NOP pressures in the same unit as PL.

5. Additional Pressure Cards

NOP - 1 cards (only if DP = 0).

6. A complete set of data cards starting with the Title Card may be put in for a new problem. A new count of points (up to 499) starts. A card containing KCL = -1 in col. 38-39 terminates the calculation.

14. Diagnostic Options

A diagnostic option KCL is provided at the end of the approximation cycle. If KCL = 9 several intermediate quantities will be printed out. (Format 20).

The first three columns contain the number ME of the point and the reduced values T_r and P_r . Then follows QZ, the mixing factor (c_{12}) for supercritical temperatures. The value ZFK obtained by the equation of Redlich and Kwong is given, then the experimental value ZE. The following column contains the value ZGG obtained by the solution of the third order equation modified by the functions L and G. The value ZG is obtained by mixing ZFK and ZGG as prescribed by QZ. The next column contains the final value ZF for the first phase obtained from ZG by addition of the deviation function DC (following column). The last column contains the numerator UP of DC.

15. Output

The first line of the output reproduces the Title Card. It is followed by the Substance Card and the T-P Schedule Cards.

If the solution of the modified cubic equation is not obtained within 0.0004 (in Z) after LAA approximation cycles, the computer prints (Format 17) the number ME of the point, the number JA of the approximation cycle, the phase distribution MTYPE of VIETA (-1 two phases, 0 critical, 1 a single phase), the factors of the cubic equation (input for VIETA), and its roots (output of VIETA).

The main output is arranged in tables for each set of temperatures and pressures. Each table starts with the following heading:

ME Number of the point for each problem.
TK Absolute temperature in °K or °R.
PA Absolute pressure in atm, psia, etc.
TR Reduced temperature.
PR Reduced pressure.
ZFK Z obtained according to Redlich and Kwong.
ZE Z observed.
ZF Z calculated.
DF Difference between ZE and ZF.

The printout for the first phase of any point may be followed by a line for a second phase.

ZSK Z for the second phase computed by the equation of Redlich and Kwong.
ZE Z observed.
ZS Z for the second phase computed by the present modified equation.
DS Difference between ZE and ZS.

If the final results from the computations do not converge within the tolerance of 0.0004 or due to some other reasons, the computer prints some number between 9.0 and 9.9.

The following is a list of the numbers which may appear in the main output rather than the actual results obtained from the calculation.

<u>Number</u>	<u>Quantity</u>	<u>Reason</u>
9.0	ZF, ZS	IA cycles do not satisfy the tolerance of 0.0004.

<u>Number</u>	<u>Quantity</u>	<u>Reason</u>
9.1	ZF, ZS	$ZFK \leq 0$.
9.2	ZF, ZS	ZC (as given in the input) > 0.333.
9.3	ZF, ZS	$T_r < 0.721$.
9.5	ZSK	only one phase is obtained from the equation of Redlich and Kwong.
9.9	ZS	The final calculation leads to a single phase.

At the critical point (and very close to it) the subroutine VIETA is insufficient. In this case inaccurate results are printed, not indicated by a printout of 9.0 or higher.

16. Phases

Since the present modified equation of state is of third order, it may furnish one or three real solutions for Z. If the equation furnishes three real solutions, the computer prints out the highest root of Z as the value for the gaseous phase and the lowest root as that for the liquid phase.

The present program does not give an indication of which of the phases is stable. This decision can be made only after the computation of the fugacity coefficients (The calculated fugacity coefficient is higher for the metastable phase).

17. Convergence

The computation of Z from the modified cubic equation is carried out by a step-by-step approximation with a damped feedback. The calculation stops either after sufficiently converging to the result or after completing a prescribed number of cycles LA without converging. The number of approximation cycles set without special instruction is 50.

More cycles can be prescribed if desired. The computer prints out the intermediate quantities for the last 10 cycles. As mentioned in Section 44, the computer does not print out the results in the main output if they do not converge except due to insufficient approximation of the VIETA feature; the number 9.0 is printed out instead.

To start the cycle, the Z value obtained from the original equation of state by Redlich and Kwong is used for the first approximation.

Oscillations of the results are suppressed by feeding back into the computation the sum of the last result multiplied by QIN, and the last-but-one result multiplied by (1-QIN). The damping factor (1-QIN) of the feedback (influence of the last-but-one result) is increased if the last two changes of the result go into opposite directions, it is decreased if the steps go into the same direction.

18. Program and Examples

In the following the complete program ES68Z as of 13 September, 1968 is reproduced.

Calculation examples are given for

Pitzer's Tables for acentric factor 0.0

0.5

Benzene (Sage and Lacey, 1955)

1-Butene (Sage and Lacey, 1955)

n-Nonane (Sage and Lacey, 1955)

Sulfur dioxide (Kang, 1961)

Hydrogen sulfide (Sage and Lacey, 1955)

Ammonia (Beattie and Lawrence, 1930)

Carbon dioxide (Sage and Lacey, 1955)

Helium (Landolt and Boernstein)

Xenon (Beattie, 1951)

Hydrogen (Landolt and Boernstein; Bartlett, 1927)

Oxygen (Michels, 1954)

The critical constants T_c , P_c and Z_c for each substance are either obtained from the quoted source of the data or from "International Critical Tables (1926-1930) or "Selected Values of Properties of Hydrocarbons and Related Compounds."

The arrangement of the output tables has been discussed in Section 45. References A, B, or C have been added to some of the output lines at the right hand side. They represent the following comments.

A. The result of this line refers to a metastable phase. Usually, though not always, the stable phase is presented in the preceding line (gas) or in the following line (liquid).

B. The calculated results for Z_c in Pitzer's Tables are 0.288 and 0.313 although the values 0.291 and 0.251 have been prescribed in the input. The subroutine VIETA cannot strictly handle the critical point. The error appears to be magnified by insufficiency of the approximation procedure. It is advisable to replace any output by a proper comment if both T_r and P_r are between 0.995 and 1.005. This has been avoided in the program so that the effect is demonstrated.

C. The input data result in $T_r < 0.721$, excluded according to Section 25.

```
PROGRAM ES64Z(INPUT,OUTPUT)
CES68 EQUATION OF STATE 1968 13 SEPT 1968
DIMENSION TI(6),SUB(4),A(4),F(4),ZE(500),P(500),TR(500),PR(500),
ZZFK(500),ZSK(500),ZF(500),ZS(500),ZG(500),X(3),Y(3),ZA(500),
3ZGG(500)
11 FORMAT (1X,6A6,3I2,2F10.4)
12 FORMAT (///)
13 FORMAT (1X,F9.4)
14 FORMAT (1X,A5,3A6,3F12.6,12)
15 FORMAT (2X,3I2,4F12.6)
16 FORMAT (19X,F12.6)
17 FORMAT (1X,3I3,7H 1ST ,5F9.4)
18 FORMAT (1X,I3,2F10.4,3(F9.3,F7.3))
19 FORMAT (10X,2(F9.3,F7.3))
20 FORMAT (1X,I3,9F6.3,F12.4)
21 FORMAT (72H NO T P TR PR ZK ZFX
2P ZCALC DIFF//)
C
C INPUT AND PREPARATION
READ 11,(TI(M),M=1,6),KCL,MCL,NPC,WOM,ECL
101 PRINT 12
PRINT 11,(TI(M),M=1,6),KCL,MCL,NPC,WOM,ECL
IF (MCL-1) 102,103,103
102 MZ=0
GO TO 104
103 MS=1
105 READ 13,ZE(ME)
IF (ZE(ME)) 101,106,131
101 ME=ME+1
GO TO 105
106 MZ=ME-1
IF (MCL-2) 104,107,108
107 MVD=0
GO TO 104
108 RP=0.016037
IF (WOM) 132,132,133
132 WOM=1.0
133 CONTINUE
MVD=-1
IF (MCL-21) 104,109,109
109 MVD=22-MCL
IF (WOM-1.0) 110,110,111
110 RP=12.1871
GO TO 112
111 RP=0.0121871
112 IF (MCL-31) 104,113,113
113 RP=0.093184
MVD=32-MCL
104 CONTINUE
READ 14,(SUB(M),M=1,4),TC,PC,ZC,LAA
PRINT 14,(SUB(M),M=1,4),TC,PC,ZC,LAA
PRINT 12
AA=ZC*ZC/5.25992106
BA=0.25992156*ZC
K=1
MX=0
114 READ 15,KS,NOT,NOP,TL,DT,PL,DP
PRINT 15,KS,NOT,NOP,TL,DT,PL,DP
P(1)=PL
JP=2
IF (DP) 115,116,117
```

```
115 P(JP)=P(JP-1)*2.0
    JP=JP+1
    IF (JP=NOP) 116,118,119
118 P(JP)=P(JP-1)*2.5
    JP=JP+1
    IF (JP=NOP) 120,120,119
120 P(JP)=P(JP-1)*2.0
    JP=JP+1
    IF (JP=NOP) 115,115,119
121 READ 16,P(JP)
    PRINT 16,P(JP)
    JP=JP+1
116 IF (JP=NOP) 121,121,119
117 P(JP)=P(JP-1)*DP
    JP=JP+1
    IF (JP=NOP) 117,117,119
119 CONTINUE
    DO 122 JT=1,NOT
    HT=FLOAT(JT)-1.0
    DO 123 JQ=1,NOP
    ME=MX+(JT-1)*NOP+JQ
    TR(ME)=(1L+HT*DT)/TC
    PR(ME)=P(JQ)/PC
123 CONTINUE
122 CONTINUE
    MX=MX+NOT*NOP
    IF (KS) 124,124,125
125 K=K+1
    GO TO 114
124 IF (LAA) 126,126,127
126 LAA=40
127 LAA=LAA+16
    IF (MZ=MX) 128,129,129
128 ML=MZ+1
    DO 130 ME=ML,MX
130 ZE(ME)=0.0
129 CONTINUE
    A(1)=1.0
    E(1)=1.0
    E(2)=-1.0
    PRINT 12
C
C M-IN CYCLE
    DO 201 ME=1,MX
    TRR=TR(ME)
    TPS=SQRT(TRR)
    TU=TRR-1.0
    PRR=PR(ME)
    IF (MCL=2) 202,203,204
203 ZE(ME)=ZE(ME)*273.15/(TRR*TC)
    GO TO 202
204 IF (MVD) 205,203,206
206 ZE(ME)=1.0/ZE(ME)
205 ZE(ME)=RR*W0*ZE(ME)*PRR*PC/(TRR*TC)
202 CONTINUE
    BIN=1.0
    IF (TRR=1.02) 209,209,210
210 UZ=1.0-EXP(-0.05/TU)
209 CONTINUE
C
R AND K
A*=0.4274*PRR/(TRR*TRR*TRS)
B*=0.08667*PRR/TRR
```

```
E(3)=AK-BK*(1.0+BK)
E(4)=-AK*BK
CALL VIETA(E,Y,MT)
ZFN(ME)=Y(1)
IF (MT) 211,211,212
211 ZSK(ME)=Y(3)
GO TO 213
212 ZSK(ME)=9.5
213 CONTINUE
AC=AA*PRR/(TRR*TRR*TRS)
EC=BA*PRR/IRR
DEN=(1.0+0.1*TRR)*(1.0+0.1*TPR)
W=0.1/(1.0+2.06*TU)
V=1.15*(1.0+2.26*TU)/DEN
U=0.103*(1.0+3.59*TU)/DEN
WA=EXP(2.30259*(1.0-3.0*ZC)/W)-1.0
ZA(1)=Y(1)
C
C APPROXIMATION CYCLE
DO 301 JA=1,LA
IF (ZA(JA)) 302,302,303
302 ZF(ME)=9.1
ZS(ME)=9.1
GO TO 201
303 D=PRR*ZC/(TRR*ZA(JA))
S=D*(3.0-D*(3.0-D))
GLL=1.0+WA*S
IF (GLL) 304,304,305
304 ZF(ME)=9.2
ZS(ME)=9.2
GO TO 201
305 GL=#*ALOG10(GLL)
IF (S-1.0) 306,307,307
306 WB=1.43/(TRR*THS)-1.32
GL=GL*(WB+(1.0-WB)*S)
307 GLG=1.0+D*S*S*(S-1.0)*(S-1.0)
IF (GLG) 308,308,309
308 ZF(ME)=9.3
ZS(ME)=9.3
GO TO 201
309 GG=#*ALOG10(GLG)
A(2)=GL-1.0
A(3)=AC*(1.0-GG)-BC*(1.0-GL+GC)
A(4)=-AC*BC*(1.0-GG)
CALL VIETA(A,X,MTYPE)
IF (JA-LAA) 312,312,313
313 PRINT 17,ME,JA,MTYPE,(A(N),N=2,4),(X(N),N=1,3)
312 ZG(ME)=X(1)
IF (ABS(ZG(ME)-ZA(JA))-0.0004) 314,325,325
325 IF (QA-10) 315,315,321
321 DIS=(X(1)-ZA(JA))*(ZA(JA)-ZA(JA-))
IF (DIS) 322,322,323
322 QIN=0.9*QIN
GO TO 315
323 QIN=QIN/0.9
IF (QIN-1.0) 315,315,324
324 QIN=1.0
315 ZA(JA+1)=QIN*ZG(ME)+(1.0-QIN)*ZA(JA)
301 CONTINUE
ZF(ME)=9.0
ZS(ME)=9.0
GO TO 201
```

```
314 ZGG(ME)=ZG(ME)
      IF (TRR-1.02) 313,310,311
311 ZG(ME)=ZFK(ME)+QZ*(ZGG(ME)-ZFK(ME))
310 CONTINUE
      IF (MTYPE) 316,317,317
317 ZS(ME)=9.9
      GO TO 318
316 ZS(ME)=X(3)
      DC=0.0
318 IF (TRR-1.02) 319,320,320
320 IT=TRR*TRR*TRR
      UP=(3.281-11.10*ZC)*(IT-2.6*TU+((4.36-15.0*ZC)*TRR-6.70+21.3*ZC)*
      2SQRT(PRR))
      DC=UP*TU*PPR/(IT*IT+0.4*PPR*PPR)
319 ZF(ME)=ZG(ME)+DC
      IF (KCL-9) 201,326,201
326 PRINT 20,ME,TRR,PPR,QZ,ZFK(ME),ZE(ME),ZGG(ME),ZG(ME),ZF(ME),DC,UP
201 CONTINUE
C
C RESULTS
PRINT 12
PRINT 21
DO 401 ME=1,MX
DF=0.0
DC=0.0
TK=TR(ME)*TC
PA=PR(ME)*PC
IF (ZF(ME)-9.0) 402,403,403
402 DF=ZE(ME)-ZF(ME)
403 PRINT 18,ME,TK,PA,TR(ME),PR(ME),ZFK(ME),ZE(ME),ZF(ME),DF
      IF (ZS(ME)) 401,401,406
406 IF (ZS(ME)-9.0) 405,401,401
405 DS=ZE(ME)-ZS(ME)
PRINT 19,ZSK(ME),ZE(ME),ZS(ME),DS
401 CONTINUE
READ 11,(TI(M),M=1,6),KCL,MCL,MPC,WOM,ECL
IF (KCL) 99,101,101
99 STOP
END
C
```

```

SUBROUTINE VIETA (A, Y, MTYPE )
SOLUTION OF THE GENERAL CUBIC EQUATION
C   A(1)*Y**3+A(2)*Y**2+A(3)*Y+A(4)=0
C   WITHOUT CUBERTF, ASINF, ACOSF, FOR GENERAL USE
DIMENSION A(4), B(3), Y(3)
B(1) = A(2)/A(1)
B10V3 = B(1)/3.0
B(2) = A(3)/A(1)
B(3) = A(4)/A(1)
ALF = B(2) - B(1)*B10V3
BET = 2.0*B10V3**3 - B(2)*B10V3 + B(3)
BETOV2 = BET/2.0
ALFOV3 = ALF/3.0
CUAOV3 = ALFOV3**3
SQBOV2 = BETOV2**2
DEL = SQBOV2 + CUAOV3
IF (DEL) 40,20,30
C
C   MTYPE=0 TWO ROOTS EQUAL
20 MTYPE = 0
GAM = SQRTF(-ALFOV3)
IF (BET) 22,22,21
21 Y(1) = -2.0*GAM -B10V3
Y(2) = GAM - B10V3
Y(3) = Y(2)
GO TO 50
22 Y(1) = 2.0*GAM -B10V3
Y(2) = -GAM -B10V3
Y(3) = Y(2)
GO TO 50
C
C   MTYPE=1 TWO COMPLEX ROOTS
30 MTYPE = 1
EPS = SQRTF(DEL)
TAU = -BETOV2
RCU=TAU+EPS
SCU=TAU-EPS
SIR=1.0
SJS=1.0
IF (RCU) 31,32,32
31 SIR=-1.0
32 IF (SCU) 33,34,34
33 SIS=-1.0
34 R=SIR*(SIR*RCU)**0.33333333
S=SJS*(SIS*SCU)**0.33333333
Y(1) = R + S - B10V3
Y(2) = -(R+S)/2.0 - B10V3
Y(3) = 0.86602540*(R-S)
GO TO 50
C
C   MTYPE=-1 THREE REAL ROOTS
40 MTYPE = -1
QUOT = SQBOV2/CUAOV3
ROOT = SQRTF(-QUOT)
IF (BET) 42,41,41
41 PHI = (1.5707963 + ATANF(ROOT / SQRTF(1.0 - ROOT**2))) / 3.0
GO TO 43
42 PHI = ATANF(SQRTF(1.0 - ROOT**2) / ROOT) / 3.0
43 FACT = 2.0*SQRTF(-ALFOV3)
Y(1) = FACT*COSEF(PHI) - B10V3
Y(2) = FACT*COSEF(PHI + 2.0943951) - B10V3

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-----
Y(3) = FACT*COSF(PHI + 4.1887902) - R10V3
C
C Y(1) HIGHEST ROOT, Y(3) LOWEST ROOT
YA=AMAX1(Y(1),Y(2),Y(3))
YC=AMIN1(Y(1),Y(2),Y(3))
YR=Y(1)+Y(2)+Y(3)-YA-YC
Y(1)=YA
Y(2)=YB
Y(3)=YC
SO RETURN
END
-----

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-----
PITZERS TABLES REDUCED          -0 1-0  -0.      -0.
ACENTRIC 0.0                    1.000000  1.000000  .291000-0
-----

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1 5 5	.800000	.100000	.200000	.400000
1 5 8	.800000	.100000	2.000000	1.000000
1 5 5	1.400000	.400000	.200000	.400000
1 5 8	1.400000	.400000	2.000000	1.000000
1 1 5	4.000000	-0.	.200000	.400000
-0 1 8	4.000000	-0.	2.000000	1.000000

NO	T	P	TR	PR	ZK	ZEXP	ZCALC	DIFF
1	.8000	.2000	.600	.200	.856	.851	.850	.001
2	.8000	.6000	.800	.600	.034	.851	.033	.818 A
3	.8000	1.0000	.800	1.000	.161	.100	.096	.004
4	.8000	1.4000	.800	1.400	.166	.164	.158	.006
5	.8000	1.8000	.800	1.800	.228	.225	.219	.006
6	.9000	.2000	.900	.200	.289	.287	.279	.008
7	.9000	.6000	.900	.600	.901	.904	.898	.006
					.597	.102	.612	-.510 A
8	.9000	1.0000	.900	1.000	.111	.102	.108	-.006
9	.9000	1.4000	.900	1.400	.175	.167	.160	.007
10	.9000	1.8000	.900	1.800	.235	.229	.220	.009
11	1.0000	.2000	1.000	.200	.294	.288	.278	.010
12	1.0000	.6000	1.000	.600	.929	.932	.931	.001
					.756	.757	.755	.002

13	1.0000	1.0000	1.000	1.000	.298	.291	.288	.003 6
14	1.0000	1.4000	1.000	1.400	.277	.250	.237	.013
15	1.0000	1.8000	1.000	1.800	.324	.304	.285	.019
16	1.1000	.2000	1.100	.200	.947	.950	.951	-.001
17	1.1000	.6000	1.100	.600	.830	.833	.831	.002
18	1.1000	1.0000	1.100	1.000	.691	.691	.682	.009
19	1.1000	1.4000	1.100	1.400	.521	.512	.498	.014
20	1.1000	1.8000	1.100	1.800	.431	.408	.411	-.003
21	1.2000	.2000	1.200	.200	.960	.963	.964	-.001
22	1.2000	.6000	1.200	.600	.875	.879	.878	.001
23	1.2000	1.0000	1.200	1.000	.785	.788	.783	.005
24	1.2000	1.4000	1.200	1.400	.693	.690	.683	.007
25	1.2000	1.8000	1.200	1.800	.612	.598	.597	.001
26	.8000	2.0000	.800	2.000	.320	.318	.311	.007
27	.8000	3.0000	.800	3.000	.466	.461	.458	.003
28	.8000	4.0000	.800	4.000	.608	.605	.600	.005
29	.8000	5.0000	.800	5.000	.746	.746	.740	.006
30	.8000	6.0000	.800	6.000	.881	.883	.876	.007
31	.8000	7.0000	.800	7.000	1.014	1.017	1.009	.008
32	.8000	8.0000	.800	8.000	1.145	1.150	1.140	.010
33	.8000	9.0000	.800	9.000	1.274	1.280	1.268	.012
34	.9000	2.0000	.900	2.000	.322	.316	.309	.007
35	.9000	3.0000	.900	3.000	.460	.458	.451	.007
36	.9000	4.0000	.900	4.000	.591	.591	.588	.003
37	.9000	5.0000	.900	5.000	.718	.718	.723	-.005
38	.9000	6.0000	.900	6.000	.841	.842	.854	-.012
39	.9000	7.0000	.900	7.000	.962	.966	.983	-.017
40	.9000	8.0000	.900	8.000	1.080	1.089	1.110	-.021
41	.9000	9.0000	.900	9.000	1.197	1.210	1.234	-.024
42	1.0000	2.0000	1.000	2.000	.349	.329	.313	.016
43	1.0000	3.0000	1.000	3.000	.472	.458	.442	.016
44	1.0000	4.0000	1.000	4.000	.592	.582	.570	.012
45	1.0000	5.0000	1.000	5.000	.707	.702	.696	.006
46	1.0000	6.0000	1.000	6.000	.820	.819	.819	-.000
47	1.0000	7.0000	1.000	7.000	.930	.932	.941	-.009
48	1.0000	8.0000	1.000	8.000	1.037	1.048	1.061	-.013
49	1.0000	9.0000	1.000	9.000	1.144	1.166	1.179	-.013
50	1.1000	2.0000	1.100	2.000	.431	.402	.409	-.007
51	1.1000	3.0000	1.100	3.000	.510	.484	.486	-.002
52	1.1000	4.0000	1.100	4.000	.610	.589	.589	-.000
53	1.1000	5.0000	1.100	5.000	.713	.699	.696	.003
54	1.1000	6.0000	1.100	6.000	.814	.810	.802	.008
55	1.1000	7.0000	1.100	7.000	.913	.916	.907	.009
56	1.1000	8.0000	1.100	8.000	1.011	1.019	1.010	.009
57	1.1000	9.0000	1.100	9.000	1.108	1.129	1.112	.017
58	1.2000	2.0000	1.200	2.000	.584	.568	.570	-.002
59	1.2000	3.0000	1.200	3.000	.576	.554	.561	-.007
60	1.2000	4.0000	1.200	4.000	.647	.618	.630	-.012
61	1.2000	5.0000	1.200	5.000	.732	.714	.717	-.003
62	1.2000	6.0000	1.200	6.000	.821	.810	.807	.003
63	1.2000	7.0000	1.200	7.000	.910	.907	.899	.008
64	1.2000	8.0000	1.200	8.000	.998	1.000	.990	.010
65	1.2000	9.0000	1.200	9.000	1.086	1.100	1.081	.019
66	1.4000	.2000	1.400	.200	.976	.977	.980	-.003
67	1.4000	.6000	1.400	.600	.927	.929	.931	-.002
68	1.4000	1.0000	1.400	1.000	.880	.883	.882	.001
69	1.4000	1.4000	1.400	1.400	.836	.838	.835	.003
70	1.4000	1.8000	1.400	1.800	.797	.795	.793	.002
71	1.8000	.2000	1.800	.200	.990	.991	.994	-.003
72	1.8000	.6000	1.800	.600	.972	.974	.977	-.003
73	1.8000	1.0000	1.800	1.000	.955	.958	.960	-.002
74	1.8000	1.4000	1.800	1.400	.941	.944	.945	-.001

75	1.8000	1.8000	1.800	1.800	.928	.931	.933	-.002
76	2.2000	.2000	2.200	.200	.996	.997	1.000	-.003
77	2.2000	.6000	2.200	.600	.989	.990	.994	-.004
78	2.2000	1.0000	2.200	1.000	.983	.984	.989	-.005
79	2.2000	1.4000	2.200	1.400	.979	.980	.985	-.005
80	2.2000	1.8000	2.200	1.800	.976	.977	.982	-.005
81	2.6000	.2000	2.600	.200	.999	1.000	1.002	-.002
82	2.6000	.6000	2.600	.600	.997	1.000	1.002	-.002
83	2.6000	1.0000	2.600	1.000	.996	1.000	1.002	-.002
84	2.6000	1.4000	2.600	1.400	.996	1.000	1.002	-.002
85	2.6000	1.8000	2.600	1.800	.997	1.002	1.004	-.002
86	3.0000	.2000	3.000	.200	1.000	1.001	1.003	-.002
87	3.0000	.6000	3.000	.600	1.001	1.003	1.005	-.002
88	3.0000	1.0000	3.000	1.000	1.003	1.005	1.008	-.003
89	3.0000	1.4000	3.000	1.400	1.005	1.008	1.010	-.002
90	3.0000	1.8000	3.000	1.800	1.008	1.012	1.014	-.002
91	1.4000	2.0000	1.400	2.000	.781	.777	.776	.001
92	1.4000	3.0000	1.400	3.000	.737	.720	.731	-.011
93	1.4000	4.0000	1.400	4.000	.753	.734	.745	-.011
94	1.4000	5.0000	1.400	5.000	.800	.781	.791	-.010
95	1.4000	6.0000	1.400	6.000	.861	.844	.851	-.007
96	1.4000	7.0000	1.400	7.000	.928	.921	.918	.003
97	1.4000	8.0000	1.400	8.000	.997	.994	.988	.006
98	1.4000	9.0000	1.400	9.000	1.068	1.071	1.060	.011
99	1.8000	2.0000	1.800	2.000	.923	.926	.927	-.001
100	1.8000	3.0000	1.800	3.000	.909	.908	.912	-.004
101	1.8000	4.0000	1.800	4.000	.911	.908	.915	-.007
102	1.8000	5.0000	1.800	5.000	.929	.925	.934	-.009
103	1.8000	6.0000	1.800	6.000	.958	.955	.963	-.008
104	1.8000	7.0000	1.800	7.000	.995	.993	1.000	-.007
105	1.8000	8.0000	1.800	8.000	1.037	1.039	1.042	-.003
106	1.8000	9.0000	1.800	9.000	1.083	1.091	1.087	.004
107	2.2000	2.0000	2.200	2.000	.975	.975	.981	-.006
108	2.2000	3.0000	2.200	3.000	.974	.974	.982	-.006
109	2.2000	4.0000	2.200	4.000	.982	.981	.991	-.010
110	2.2000	5.0000	2.200	5.000	.997	.997	1.007	-.010
111	2.2000	6.0000	2.200	6.000	1.017	1.020	1.030	-.010
112	2.2000	7.0000	2.200	7.000	1.043	1.048	1.058	-.010
113	2.2000	8.0000	2.200	8.000	1.073	1.080	1.088	-.008
114	2.2000	9.0000	2.200	9.000	1.105	1.118	1.122	-.004
115	2.6000	2.0000	2.600	2.000	.998	1.003	1.005	-.002
116	2.6000	3.0000	2.600	3.000	1.004	1.010	1.012	-.002
117	2.6000	4.0000	2.600	4.000	1.015	1.023	1.025	-.002
118	2.6000	5.0000	2.600	5.000	1.029	1.040	1.041	-.001
119	2.6000	6.0000	2.600	6.000	1.047	1.059	1.062	-.003
120	2.6000	7.0000	2.600	7.000	1.068	1.083	1.085	-.002
121	2.6000	8.0000	2.600	8.000	1.092	1.109	1.111	-.002
122	2.6000	9.0000	2.600	9.000	1.118	1.139	1.139	.000
123	3.0000	2.0000	3.000	2.000	1.009	1.014	1.016	-.002
124	3.0000	3.0000	3.000	3.000	1.019	1.028	1.026	.002
125	3.0000	4.0000	3.000	4.000	1.031	1.041	1.040	.001
126	3.0000	5.0000	3.000	5.000	1.045	1.058	1.057	.001
127	3.0000	6.0000	3.000	6.000	1.062	1.077	1.076	.001
128	3.0000	7.0000	3.000	7.000	1.080	1.100	1.097	.002
129	3.0000	8.0000	3.000	8.000	1.101	1.124	1.119	.002
130	3.0000	9.0000	3.000	9.000	1.123	1.150	1.144	.006
131	4.0000	.2000	4.000	.200	1.002	1.003	1.004	-.001
132	4.0000	.6000	4.000	.600	1.005	1.005	1.008	-.003
133	4.0000	1.0000	4.000	1.000	1.009	1.013	1.013	.000
134	4.0000	1.4000	4.000	1.400	1.013	1.017	1.017	-.000
135	4.0000	1.8000	4.000	1.800	1.017	1.022	1.022	.000
136	4.0000	2.0000	4.000	2.000	1.019	1.024	1.024	-.000

33	.8000	9.0000	.800	9.000	1.274	1.105	1.100	.605
34	.9000	2.0000	.900	2.000	.322	.246	.278	-.032
35	.9000	3.0000	.900	3.000	.460	.368	.400	-.032
36	.9000	4.0000	.900	4.000	.591	.486	.518	-.032
37	.9000	5.0000	.900	5.000	.718	.598	.634	-.036
38	.9000	6.0000	.900	6.000	.841	.707	.747	-.040
39	.9000	7.0000	.900	7.000	.962	.816	.858	-.042
40	.9000	8.0000	.900	8.000	1.080	.929	.967	-.038
41	.9000	9.0000	.900	9.000	1.197	1.035	1.074	-.039
42	1.0000	2.0000	1.000	2.000	.349	.267	.281	-.014
43	1.0000	3.0000	1.000	3.000	.472	.383	.392	-.009
44	1.0000	4.0000	1.000	4.000	.592	.497	.503	-.006
45	1.0000	5.0000	1.000	5.000	.707	.602	.611	-.009
46	1.0000	6.0000	1.000	6.000	.820	.704	.718	-.014
47	1.0000	7.0000	1.000	7.000	.930	.802	.823	-.021
48	1.0000	8.0000	1.000	8.000	1.037	.898	.926	-.028
49	1.0000	9.0000	1.000	9.000	1.144	1.001	1.027	-.026
50	1.1000	2.0000	1.100	2.000	.431	.402	.390	.012
51	1.1000	3.0000	1.100	3.000	.510	.449	.456	-.007
52	1.1000	4.0000	1.100	4.000	.610	.539	.551	-.012
53	1.1000	5.0000	1.100	5.000	.713	.634	.649	-.015
54	1.1000	6.0000	1.100	6.000	.814	.730	.748	-.018
55	1.1000	7.0000	1.100	7.000	.913	.811	.846	-.035
56	1.1000	8.0000	1.100	8.000	1.011	.894	.942	-.048
57	1.1000	9.0000	1.100	9.000	1.108	.989	1.038	-.049
58	1.2000	2.0000	1.200	2.000	.584	.653	.565	.088
59	1.2000	3.0000	1.200	3.000	.576	.589	.549	.040
60	1.2000	4.0000	1.200	4.000	.647	.618	.609	.009
61	1.2000	5.0000	1.200	5.000	.732	.694	.687	.007
62	1.2000	6.0000	1.200	6.000	.821	.770	.772	-.002
63	1.2000	7.0000	1.200	7.000	.910	.847	.858	-.011
64	1.2000	8.0000	1.200	8.000	.998	.920	.945	-.025
65	1.2000	9.0000	1.200	9.000	1.086	1.005	1.031	-.026
66	1.4000	.2000	1.400	.200	.976	.985	.992	-.007
67	1.4000	.6000	1.400	.600	.927	.954	.952	.002
68	1.4000	1.0000	1.400	1.000	.880	.924	.909	.015
69	1.4000	1.4000	1.400	1.400	.836	.903	.865	.038
70	1.4000	1.8000	1.400	1.800	.797	.885	.823	.062
71	1.8000	.2000	1.800	.200	.990	1.000	1.006	-.006
72	1.8000	.6000	1.800	.600	.972	1.001	1.002	-.001
73	1.8000	1.0000	1.800	1.000	.955	1.003	.998	.005
74	1.8000	1.4000	1.800	1.400	.941	.999	.995	.004
75	1.8000	1.8000	1.800	1.800	.928	1.006	.994	.012
76	2.2000	.2000	2.200	.200	.996	1.004	1.011	-.007
77	2.2000	.6000	2.200	.600	.989	1.013	1.018	-.005
78	2.2000	1.0000	2.200	1.000	.983	1.022	1.027	-.005
79	2.2000	1.4000	2.200	1.400	.979	1.033	1.036	-.003
80	2.2000	1.8000	2.200	1.800	.976	1.043	1.046	-.003
81	2.6000	.2000	2.600	.200	.999	1.005	1.012	-.007
82	2.6000	.6000	2.600	.600	.997	1.019	1.023	-.004
83	2.6000	1.0000	2.600	1.000	.996	1.034	1.035	-.001
84	2.6000	1.4000	2.600	1.400	.996	1.048	1.048	-.000
85	2.6000	1.8000	2.600	1.800	.997	1.060	1.062	-.002
86	3.0000	.2000	3.000	.200	1.000	1.006	1.012	-.006
87	3.0000	.6000	3.000	.600	1.001	1.018	1.024	-.006
88	3.0000	1.0000	3.000	1.000	1.003	1.035	1.037	-.002
89	3.0000	1.4000	3.000	1.400	1.005	1.048	1.050	-.002
90	3.0000	1.8000	3.000	1.800	1.008	1.062	1.064	-.002
91	1.4000	2.0000	1.400	2.000	.781	.872	.805	.067
92	1.4000	3.0000	1.400	3.000	.737	.820	.759	.061
93	1.4000	4.0000	1.400	4.000	.753	.809	.768	.041
94	1.4000	5.0000	1.400	5.000	.800	.836	.807	.029

95	1.4000	6.0000	1.400	6.000	.861	.879	.859	.020
96	1.4000	7.0000	1.400	7.000	.928	.941	.919	.022
97	1.4000	8.0000	1.400	8.000	.997	.999	.983	.016
98	1.4000	9.0000	1.400	9.000	1.066	1.066	1.049	.017
99	1.8000	2.0000	1.800	2.000	.923	1.006	.993	.013
100	1.8000	3.0000	1.800	3.000	.909	1.013	1.001	.012
101	1.8000	4.0000	1.800	4.000	.911	1.038	1.023	.015
102	1.8000	5.0000	1.800	5.000	.929	1.070	1.056	.014
103	1.8000	6.0000	1.800	6.000	.958	1.110	1.094	.016
104	1.8000	7.0000	1.800	7.000	.995	1.153	1.135	.018
105	1.8000	8.0000	1.800	8.000	1.037	1.199	1.179	.020
106	1.8000	9.0000	1.800	9.000	1.083	1.241	1.223	.018
107	2.2000	2.0000	2.200	2.000	.975	1.046	1.051	-.005
108	2.2000	3.0000	2.200	3.000	.974	1.077	1.083	-.006
109	2.2000	4.0000	2.200	4.000	.982	1.109	1.121	-.012
110	2.2000	5.0000	2.200	5.000	.997	1.147	1.166	-.019
111	2.2000	6.0000	2.200	6.000	1.017	1.195	1.214	-.019
112	2.2000	7.0000	2.200	7.000	1.043	1.248	1.264	-.016
113	2.2000	8.0000	2.200	8.000	1.073	1.299	1.315	-.016
114	2.2000	9.0000	2.200	9.000	1.105	1.353	1.365	-.012
115	2.6000	2.0000	2.600	2.000	.998	1.066	1.069	-.003
116	2.6000	3.0000	2.600	3.000	1.004	1.107	1.106	.001
117	2.6000	4.0000	2.600	4.000	1.015	1.146	1.148	-.002
118	2.6000	5.0000	2.600	5.000	1.029	1.188	1.194	-.006
119	2.6000	6.0000	2.600	6.000	1.047	1.233	1.244	-.011
120	2.6000	7.0000	2.600	7.000	1.068	1.281	1.295	-.014
121	2.6000	8.0000	2.600	8.000	1.092	1.334	1.348	-.014
122	2.6000	9.0000	2.600	9.000	1.118	1.389	1.401	-.012
123	3.0000	2.0000	3.000	2.000	1.009	1.069	1.072	-.003
124	3.0000	3.0000	3.000	3.000	1.019	1.113	1.109	.004
125	3.0000	4.0000	3.000	4.000	1.031	1.156	1.150	.006
126	3.0000	5.0000	3.000	5.000	1.045	1.198	1.193	.005
127	3.0000	6.0000	3.000	6.000	1.062	1.247	1.239	.008
128	3.0000	7.0000	3.000	7.000	1.080	1.290	1.287	.003
129	3.0000	8.0000	3.000	8.000	1.101	1.349	1.336	.013
130	3.0000	9.0000	3.000	9.000	1.123	1.400	1.386	.014
131	4.0000	2.0000	4.000	2.000	1.002	1.008	1.010	-.002
132	4.0000	3.0000	4.000	3.000	1.005	1.015	1.021	-.006
133	4.0000	4.0000	4.000	4.000	1.009	1.033	1.033	.000
134	4.0000	5.0000	4.000	5.000	1.013	1.047	1.045	.002
135	4.0000	6.0000	4.000	6.000	1.017	1.057	1.057	.000
136	4.0000	7.0000	4.000	7.000	1.019	1.064	1.063	.001
137	4.0000	8.0000	4.000	8.000	1.031	1.098	1.095	.003
138	4.0000	9.0000	4.000	9.000	1.043	1.133	1.127	.006
139	4.0000	1.0000	4.000	1.000	1.057	1.168	1.161	.007
140	4.0000	2.0000	4.000	2.000	1.071	1.201	1.196	.005
141	4.0000	3.0000	4.000	3.000	1.087	1.239	1.232	.007
142	4.0000	4.0000	4.000	4.000	1.103	1.279	1.269	.010
143	4.0000	5.0000	4.000	5.000	1.119	1.318	1.307	.011

SAGE AND LACEY ZEXP -C 1-0 -0. -0.
 BENZENE RANKINE PSI 1912.700000 714.000000 .274000-0

1 2 2 559.680000 189.000000 200.000000 400.000000
 1 1 1 919.680000 -0. 600.000000 -0.
 -0 3 4 559.680000 189.000000 1000.000000 -1.000000

NO	T	P	TR	PR	ZK	ZEXP	ZCALC	DIFF
1	559.6800	200.0000	.553	.280	.054	.048	9.300	0. C
2	559.6800	600.0000	.553	.840	.161	.145	9.300	0. C
3	739.6800	200.0000	.730	.280	.685	.042	.679	-.637
					.048	.042	.041	.000
4	739.6800	600.0000	.730	.840	.141	.125	.117	.008
5	919.6800	600.0000	.908	.840	.151	.125	.128	-.002
6	559.6800	1000.0000	.553	1.401	.266	.240	9.300	0. C
7	559.6800	2000.0000	.553	2.801	.527	.477	9.300	0. C
8	559.6800	5000.0000	.553	7.003	1.287	1.170	9.300	0. C
9	559.6800	10000.0000	.553	14.006	2.505	2.286	9.300	0. C
10	739.6800	1000.0000	.730	1.401	.232	.206	.193	.013
11	739.6800	2000.0000	.730	2.801	.451	.406	.378	.028
12	739.6800	5000.0000	.730	7.003	1.066	.980	.902	.078
13	739.6800	10000.0000	.730	14.006	2.024	1.880	1.709	.171
14	919.6800	1000.0000	.908	1.401	.237	.203	.206	-.003
15	919.6800	2000.0000	.908	2.801	.433	.386	.395	-.004
16	919.6800	5000.0000	.908	7.003	.959	.890	.919	-.029
17	919.6800	10000.0000	.908	14.006	1.752	1.660	1.713	-.053

SAGE AND LACEY ZEXP -0 1-0 -0. -0.
 1-BUTENE RANKINE PSIA 756.680000 588.000000 .279000-0

1 3 5 559.680000 120.000000 200.000000 200.000000
 -0 3 9 559.680000 120.000000 2000.000000 1000.000000

NO	T	P	TR	PR	ZK	ZEXP	ZCALC	DIFF
1	559.6800	200.0000	.740	.340	.564	.052	.599	-.546
					.058	.052	.050	.002
2	559.6800	400.0000	.740	.680	.114	1.044	.099	.945
3	559.6800	600.0000	.740	1.020	.170	.156	.148	.008
4	559.6800	800.0000	.740	1.361	.225	.207	.196	.011
5	559.6800	1000.0000	.740	1.701	.279	.257	.243	.014
6	679.6800	200.0000	.898	.340	.818	.812	.811	.001
7	679.6800	400.0000	.898	.680	.123	.106	.467	-.362
					9.500	.106	.110	-.004
8	679.6800	600.0000	.898	1.020	.177	.156	.156	.001
9	679.6800	800.0000	.898	1.361	.229	.206	.205	.001
10	679.6800	1000.0000	.898	1.701	.279	.254	.253	.001
11	799.6800	200.0000	1.057	.340	.895	.901	.899	.002
12	799.6800	400.0000	1.057	.680	.772	.778	.770	.006
13	799.6800	600.0000	1.057	1.020	.612	.618	.593	.025
14	799.6800	800.0000	1.057	1.361	.390	.393	.356	.037
15	799.6800	1000.0000	1.057	1.701	.363	.327	.328	-.001
16	559.6800	2000.0000	.740	3.401	.539	.504	.477	.027
17	559.6800	3000.0000	.740	5.102	.789	.745	.700	.045
18	559.6800	4000.0000	.740	6.803	1.031	.980	.915	.065

19	559.6800	5000.0000	.740	8.503	1.267	1.210	1.125	.085
20	559.6800	6000.0000	.740	10.204	1.499	1.434	1.329	.165
21	559.6800	7000.0000	.740	11.905	1.728	1.657	1.529	.128
22	559.6800	8000.0000	.740	13.605	1.953	1.875	1.725	.150
23	559.6800	9000.0000	.740	15.306	2.177	2.092	1.918	.174
24	559.6800	10000.0000	.740	17.007	2.398	2.307	2.107	.200
25	679.6800	2000.0000	.898	3.401	.513	.482	.485	-.003
26	679.6800	3000.0000	.898	5.102	.731	.697	.705	-.008
27	679.6800	4000.0000	.898	6.803	.939	.905	.918	-.013
28	679.6800	5000.0000	.898	8.503	1.140	1.108	1.123	-.015
29	679.6800	6000.0000	.898	10.204	1.337	1.307	1.324	-.017
30	679.6800	7000.0000	.898	11.905	1.529	1.502	1.519	-.017
31	679.6800	8000.0000	.898	13.605	1.719	1.691	1.710	-.019
32	679.6800	9000.0000	.898	15.306	1.907	1.878	1.896	-.018
33	679.6800	10000.0000	.898	17.007	2.092	2.062	2.077	-.015
34	799.6800	2000.0000	1.057	3.401	.534	.511	.495	.016
35	799.6800	3000.0000	1.057	5.102	.719	.700	.685	.015
36	799.6800	4000.0000	1.057	6.803	.898	.884	.871	.013
37	799.6800	5000.0000	1.057	8.503	1.072	1.061	1.053	.008
38	799.6800	6000.0000	1.057	10.204	1.241	1.236	1.230	.006
39	799.6800	7000.0000	1.057	11.905	1.407	1.408	1.404	.004
40	799.6800	8000.0000	1.057	13.605	1.570	1.577	1.574	.003
41	799.6800	9000.0000	1.057	15.306	1.731	1.742	1.742	.000
42	799.6800	10000.0000	1.057	17.007	1.889	1.903	1.906	-.003

SAGE AND LACEY CU FT PER LB MOLE -033-0 -0. -0.
 N=NONANE RANKINE PSIA 1570.210000 332.000000 .254000-0

1 4 5 559.680000 120.000000 200.000000 200.000000
 -0 4 9 559.680000 120.000000 2000.000000 1000.000000

NO	T	P	TR	PR	ZK	ZEXP	ZCALC	DIFF
1	559.6800	200.0000	.523	.602	.120	.097	9.300	0. C
2	559.6800	400.0000	.523	1.205	.238	.193	9.300	0. C
3	559.6800	600.0000	.523	1.807	.356	.290	9.300	0. C
4	559.6800	800.0000	.523	2.410	.473	.386	9.300	0. C
5	559.6800	1000.0000	.523	3.012	.589	.481	9.300	0. C
6	679.6800	200.0000	.635	.602	.107	.086	9.300	0. C
7	679.6800	400.0000	.635	1.205	.212	.172	9.300	0. C
8	679.6800	600.0000	.635	1.807	.315	.257	9.300	0. C
9	679.6800	800.0000	.635	2.410	.417	.342	9.300	0. C
10	679.6800	1000.0000	.635	3.012	.518	.428	9.300	0. C
11	799.6800	200.0000	.747	.602	.101	.081	.078	.002
12	799.6800	400.0000	.747	1.205	.199	.161	.157	.004
13	799.6800	600.0000	.747	1.807	.294	.240	.234	.006
14	799.6800	800.0000	.747	2.410	.387	.318	.310	.008
15	799.6800	1000.0000	.747	3.012	.479	.395	.384	.011
16	919.6800	200.0000	.859	.602	.105	.080	.477	-.397A
17	919.6800	400.0000	.859	1.205	9.500	.080	.087	-.007
18	919.6800	600.0000	.859	1.807	.200	.158	.165	-.007
19	919.6800	800.0000	.859	2.410	.291	.234	.244	-.010
					.378	.309	.320	-.011

20	919.6000	1000.0000	.859	3.012	.462	.382	.395	-.013
21	559.6000	2000.0000	.523	6.024	1.159	.954	9.300	0.
22	559.6000	3000.0000	.523	9.036	1.718	1.419	9.300	0.
23	559.6000	4000.0000	.523	12.048	2.277	1.877	9.300	0.
24	559.6000	5000.0000	.523	15.060	2.810	2.330	9.300	0.
25	559.6000	6000.0000	.523	18.072	3.347	2.778	9.300	0.
26	559.6000	7000.0000	.523	21.084	3.880	3.223	9.300	0.
27	559.6000	8000.0000	.523	24.096	4.409	3.670	9.300	0.
28	559.6000	9000.0000	.523	27.108	4.935	4.112	9.300	0.
29	559.6000	10000.0000	.523	30.120	5.459	4.545	9.300	0.
30	679.6000	2000.0000	.635	6.024	1.010	.845	9.300	0.
31	679.6000	3000.0000	.635	9.036	1.484	1.250	9.300	0.
32	679.6000	4000.0000	.635	12.048	1.948	1.651	9.300	0.
33	679.6000	5000.0000	.635	15.060	2.404	2.043	9.300	0.
34	679.6000	6000.0000	.635	18.072	2.853	2.432	9.300	0.
35	679.6000	7000.0000	.635	21.084	3.298	2.817	9.300	0.
36	679.6000	8000.0000	.635	24.096	3.739	3.198	9.300	0.
37	679.6000	9000.0000	.635	27.108	4.176	3.572	9.300	0.
38	679.6000	10000.0000	.635	30.120	4.611	3.938	9.300	0.
39	799.6000	2000.0000	.747	6.024	.916	.774	.744	.029
40	799.6000	3000.0000	.747	9.036	1.332	1.140	1.083	.057
41	799.6000	4000.0000	.747	12.048	1.735	1.496	1.406	.090
42	799.6000	5000.0000	.747	15.060	2.129	1.847	1.718	.129
43	799.6000	6000.0000	.747	18.072	2.515	2.188	2.021	.167
44	799.6000	7000.0000	.747	21.084	2.899	2.520	2.317	.204
45	799.6000	8000.0000	.747	24.096	3.277	2.862	2.606	.256
46	799.6000	9000.0000	.747	27.108	3.652	3.188	2.891	.297
47	799.6000	10000.0000	.747	30.120	4.025	3.519	3.172	.347
48	919.6000	2000.0000	.859	6.024	.858	.734	.754	-.020
49	919.6000	3000.0000	.859	9.036	1.229	1.070	1.091	-.021
50	919.6000	4000.0000	.859	12.048	1.586	1.394	1.413	-.019
51	919.6000	5000.0000	.859	15.060	1.934	1.712	1.721	-.009
52	919.6000	6000.0000	.859	18.072	2.275	2.018	2.018	.001
53	919.6000	7000.0000	.859	21.084	2.611	2.319	2.305	.014
54	919.6000	8000.0000	.859	24.096	2.942	2.618	2.584	.034
55	919.6000	9000.0000	.859	27.108	3.271	2.909	2.855	.054
56	919.6000	10000.0000	.859	30.120	3.597	3.202	3.121	.081

KANG CHEM ENG DATA 6 1961 ZE (P -0 1-0 -0, -0.
 SULFLF CIG4IDE K PSI 430.650000 77.803000 .269700-0

1 2 3	323.150000	50.000000	2.000000	3.000000
1 2 2	423.150000	7.500000	10.000000	11.000000
1 1 2	373.150000	-0.	14.000000	17.000000
1 1 4	423.150000	-0.	30.000000	17.000000
1 1 3	430.650000	-0.	50.000000	7.000000
-0 2 4	430.650000	32.500000	75.000000	77.000000

NC	I	P	FR	PR	ZK	ZE 4P	ZCALC	DIFF
1	323.1500	2.0000	.750	.026	.981	.974	.972	.002
					.004	.974	.004	.970 A
2	323.1500	5.0000	.750	.064	.949	.934	.933	.002
					.011	.934	.011	.924 A
3	323.1500	8.0000	.750	.103	.911	.851	.874	.004
					.018	.891	.015	.874 A
4	373.1500	2.0000	.366	.026	.987	.985	.979	.006
5	373.1500	5.0000	.366	.064	.951	.962	.953	.009
6	373.1500	8.0000	.366	.103	.941	.939	.928	.010
7	423.1500	10.0000	.933	.129	.951	.950	.947	.003
8	423.1500	20.0000	.933	.257	.901	.877	.896	.001
9	430.6500	10.0000	1.000	.129	.951	.953	.952	.001
10	430.6500	20.0000	1.000	.257	.901	.904	.904	.000
11	373.1500	14.0000	.366	.180	.901	.887	.881	.005

12	273.1500	25.0000	.965	.334	.791	.761	.783	-.022
13	223.1500	30.0000	.983	.356	.841	.839	.841	-.001
14	223.1500	40.0000	.983	.514	.784	.774	.778	-.005
15	223.1500	50.0000	.983	.643	.711	.698	.706	-.008
16	223.1500	60.0000	.983	.771	.624	.600	.615	-.015
17	230.6500	50.0000	1.000	.643	.734	.724	.726	-.002
18	230.6500	100.0000	1.000	1.285	.261	.215	.208	.007
19	230.6500	250.0000	1.000	3.213	.491	.436	.432	.004
20	230.6500	75.0000	1.000	.964	.471	.447	.449	-.002
21	230.6500	150.0000	1.000	1.928	.340	.287	.278	.009
22	230.6500	225.0000	1.000	2.892	.451	.402	.394	.008
23	230.6500	300.0000	1.000	3.856	.571	.509	.508	.000
24	223.1500	75.0000	1.215	.964	.801	.823	.809	.014
25	223.1500	150.0000	1.215	1.928	.614	.646	.601	.045
26	223.1500	225.0000	1.215	2.892	.584	.576	.568	.008
27	223.1500	300.0000	1.215	3.856	.641	.615	.620	-.005

SAGE AND LACEY ZEXP -0 1-0 -0. -0.
 HYDROGEN SULFIDE R PSI 671.93000 1306.00000 .2633 00-0

1 1 7 499.68000 -0. 100.00000 -0.00000
 -0 2 7 559.68000 120.00000 100.00000 -0.00000

NO	I	P	IR	PR	ZK	ZEXP	ZCALC	DIFF
1	499.6800	100.0000	.744	.077	.937	.922	.928	-.006
2	499.6800	200.0000	.744	.153	.851	.825	.854	-.029
3	499.6800	500.0000	.744	.383	.621	.625	.624	.000
4	499.6800	1000.0000	.744	.766	.501	.661	.477	-.016
5	499.6800	2000.0000	.744	1.531	.251	.661	.056	.005
6	499.6800	5000.0000	.744	3.823	.251	.240	.114	.007
7	499.6800	10000.0000	.744	7.657	.601	.515	.225	.015
8	559.6800	100.0000	.833	.077	1.141	1.114	.544	.035
9	559.6800	200.0000	.833	.153	1.041	1.041	.073	.003
10	559.6800	500.0000	.833	.383	.951	.950	.947	.003
11	559.6800	1000.0000	.833	.766	.901	.898	.896	.003
12	559.6800	2000.0000	.833	1.531	.821	.898	.031	.867
13	559.6800	5000.0000	.833	3.823	.021	.898	.031	.867
14	559.6800	10000.0000	.833	7.657	.061	.898	.031	.867
15	679.6800	100.0000	1.011	.077	.717	.661	.717	-.656
16	679.6800	200.0000	1.011	.153	.061	.661	.063	-.002
17	679.6800	500.0000	1.011	.383	.121	.661	.119	.001
18	679.6800	1000.0000	1.011	.766	.121	.661	.119	.001
19	679.6800	2000.0000	1.011	1.531	.241	.224	.233	.001
20	679.6800	5000.0000	1.011	3.823	.577	.554	.556	-.003
21	679.6800	10000.0000	1.011	7.657	1.071	1.052	1.058	-.006
22	799.6800	100.0000	1.190	.077	.971	.974	.975	-.001
23	799.6800	200.0000	1.190	.153	.941	.948	.949	-.001
24	799.6800	500.0000	1.190	.383	.861	.864	.863	.001
25	799.6800	1000.0000	1.190	.766	.691	.678	.670	.008
26	799.6800	2000.0000	1.190	1.531	.301	.265	.250	.015
27	799.6800	5000.0000	1.190	3.823	.571	.545	.530	.015
28	799.6800	10000.0000	1.190	7.657	.997	.973	.985	-.012
29	799.6800	100.0000	1.190	.077	.984	.985	.988	-.003
30	799.6800	200.0000	1.190	.153	.961	.971	.974	-.003

24	799.6800	500.0000	1.190	.383	.919	.925	.926	-.001
25	799.6800	1000.0000	1.190	.766	.839	.844	.837	.008
26	799.6800	2000.0000	1.190	1.531	.650	.657	.638	.019
27	799.6800	5000.0000	1.190	3.828	.629	.597	.609	-.012
28	799.6800	10000.0000	1.190	7.657	.968	.946	.953	-.006

BEATTIE AND LAWRENCE CC PER GRAM -023-0 17.0210 -9.
 AMMONIA KELVIN ATM 405.550000 111.500000 .242500-0

1	1	1	323.150000	-0.	1.137000	-(-.
1	1	1	323.150000	-0.	4.935000	-(-.
1	1	1	323.150000	-0.	9.567000	-(-.
1	1	1	323.150000	-0.	14.370000	-(-.
1	1	1	323.150000	-0.	15.050000	-(-.
1	1	1	323.150000	-0.	15.722000	-(-.
1	1	1	323.150000	-0.	16.620000	-(-.
1	1	1	323.150000	-0.	18.540000	-(-.
1	1	1	373.150000	-0.	1.374000	-(-.
1	1	1	373.150000	-0.	5.832000	-(-.
1	1	1	373.150000	-0.	11.352000	-(-.
1	1	1	373.150000	-0.	17.360000	-(-.
1	1	1	373.150000	-0.	19.109000	-(-.
1	1	1	373.150000	-0.	20.290000	-(-.
1	1	1	373.150000	-0.	26.120000	-(-.
1	1	1	373.150000	-0.	36.470000	-(-.
1	1	1	373.150000	-0.	45.190000	-(-.
1	1	1	373.150000	-0.	51.090000	-(-.
1	1	1	373.150000	-0.	58.280000	-(-.
1	1	1	473.150000	-0.	1.747000	-(-.
1	1	1	473.150000	-0.	7.489000	-(-.
1	1	1	473.150000	-0.	14.766000	-(-.
1	1	1	473.150000	-0.	22.930000	-(-.
1	1	1	473.150000	-0.	25.361000	-(-.
1	1	1	473.150000	-0.	27.010000	-(-.
1	1	1	473.150000	-0.	35.400000	-(-.
1	1	1	473.150000	-0.	51.290000	-(-.
1	1	1	473.150000	-0.	66.050000	-(-.
1	1	1	473.150000	-0.	77.130000	-(-.
1	1	1	473.150000	-0.	92.570000	-(-.
1	1	1	593.150000	-0.	29.590000	-(-.
1	1	1	593.150000	-0.	35.040000	-(-.
1	1	1	593.150000	-0.	45.340000	-(-.
1	1	1	593.150000	-0.	63.360000	-(-.
1	1	1	593.150000	-0.	83.690000	-(-.
1	1	1	593.150000	-0.	106.250000	-(-.
-0	1	1	593.150000	-0.	130.400000	-(-.

NO	T	P	TR	PR	ZK	ZE (P	ZCALC	DIFF
1	323.1500	1.1870	.797	.011	.999	.991	.978	.013
2	323.1500	4.9850	.797	.045	.971	.961	.932	.028
3	323.1500	9.5670	.797	.086	.947	.922	.891	.031
4	323.1500	14.3700	.797	.129	.911	.877	.853	.024

5	223.1500	15.0500	.797	.135	.901	.810	.847	.023
6	223.1500	15.7220	.797	.141	.901	.863	.842	.021
7	223.1500	16.6200	.797	.149	.891	.854	.836	.018
8	223.1500	18.5400	.797	.166	.881	.834	.821	.012
9	273.1500	1.3740	.920	.012	.991	.954	.979	.015
10	273.1500	5.8320	.920	.052	.971	.973	.949	.025
11	273.1500	11.3520	.920	.102	.951	.947	.922	.025
12	273.1500	17.3600	.920	.156	.921	.917	.895	.022
13	273.1500	19.1090	.920	.171	.921	.909	.888	.021
14	273.1500	20.2800	.920	.182	.911	.902	.883	.020
15	273.1500	24.1200	.920	.234	.891	.872	.857	.014
16	273.1500	36.4700	.920	.327	.841	.811	.810	.001
17	273.1500	45.1900	.920	.405	.791	.754	.768	-.014
18	273.1500	51.0900	.920	.458	.761	.710	.737	-.026
19	273.1500	58.2800	.920	.523	.711	.648	.696	-.047
20	473.1500	1.7470	1.167	.015	.991	.996	1.003	-.007
21	473.1500	7.4890	1.167	.067	.981	.986	.996	-.010
22	473.1500	14.7650	1.167	.132	.971	.972	.984	-.013
23	473.1500	22.9300	1.167	.206	.951	.956	.970	-.014
24	473.1500	25.3610	1.167	.227	.951	.951	.965	-.014
25	473.1500	27.0100	1.167	.242	.941	.948	.962	-.014
26	473.1500	35.4000	1.167	.317	.921	.932	.946	-.014
27	473.1500	51.2900	1.167	.460	.891	.900	.913	-.013
28	473.1500	66.0500	1.167	.592	.861	.869	.881	-.011
29	473.1500	77.1300	1.167	.692	.831	.846	.855	-.009
30	473.1500	92.5700	1.167	.830	.801	.812	.816	-.004
31	598.1500	29.5900	1.475	.265	.971	.975	.995	-.019
32	598.1500	35.0400	1.475	.314	.961	.973	.991	-.019
33	598.1500	46.3400	1.475	.416	.951	.965	.985	-.020
34	598.1500	68.3500	1.475	.613	.931	.949	.971	-.022
35	598.1500	85.6900	1.475	.804	.911	.934	.957	-.023
36	598.1500	106.2500	1.475	.953	.901	.922	.945	-.024
37	598.1500	130.4000	1.475	1.170	.881	.905	.929	-.024

SAGE END LACEY ZEXP -0.1-0 -0. -0.
 CARBON DIOXIDE R PSI 547.430000 1059.870000 .274500-0

1 1 2 499.680000 -0. 200.000000 401.000000
 1 4 2 559.680000 120.000000 200.000000 401.000000
 1 1 4 499.680000 -0. 1000.000000 -1.000000
 -0 4 4 559.680000 120.000000 1000.000000 -1.000000

NO	I	P	FR	PR	ZK	ZEXP	ZCALC	DIFF
1	499.6800	200.0000	.913	.187	.911	.906	.945	-.039
2	499.6800	600.0000	.913	.561	.851	.887	.714	-.627
3	559.6800	200.0000	1.022	.187	.931	.938	.940	-.002
4	559.6800	600.0000	1.022	.561	.791	.793	.792	.001
5	679.6800	200.0000	1.241	.187	.961	.968	.975	-.005
6	679.6800	600.0000	1.241	.561	.891	.804	.906	-.002
7	799.6800	200.0000	1.461	.187	.981	.983	.989	-.005
8	799.6800	600.0000	1.461	.561	.941	.951	.954	-.003
9	819.6800	200.0000	1.680	.187	.991	.992	.997	-.005

10	119.6800	600.0000	1.580	.561	.961	.976	.979	-.004
11	199.6800	1000.0000	.913	.935	.161	.143	.152	-.009
12	199.6800	2000.0000	.913	1.869	.301	.275	.282	-.007
13	199.6800	5000.0000	.913	4.673	.671	.623	.645	-.022
14	199.6800	10000.0000	.913	9.347	1.221	1.160	1.205	-.044
15	159.6800	1000.0000	1.022	.935	.581	.587	.566	.020
16	159.6800	2000.0000	1.022	1.869	.341	.302	.290	.012
17	159.6800	5000.0000	1.022	4.673	.671	.624	.616	.003
18	159.6800	10000.0000	1.022	9.347	1.171	1.120	1.137	-.017
19	119.6800	1000.0000	1.241	.935	.921	.839	.831	.003
20	119.6800	2000.0000	1.241	1.869	.651	.681	.647	.034
21	119.6800	5000.0000	1.241	4.673	.711	.695	.697	-.002
22	119.6800	10000.0000	1.241	9.347	1.101	1.087	1.087	.000
23	199.6800	1000.0000	1.461	.935	.901	.820	.819	.001
24	199.6800	2000.0000	1.461	1.869	.821	.853	.837	.016
25	199.6800	5000.0000	1.461	4.673	.801	.825	.816	.009
26	199.6800	10000.0000	1.461	9.347	1.091	1.102	1.085	.017
27	119.6800	1000.0000	1.680	.935	.941	.960	.962	-.002
28	119.6800	2000.0000	1.680	1.869	.901	.930	.925	.005
29	119.6800	5000.0000	1.680	4.673	.881	.925	.925	.001
30	119.6800	10000.0000	1.680	9.347	1.091	1.127	1.123	.004

LANDOLT AND BOERNSTEIN, AMAGAT -0.2-0 -0. -0.
 HELIUM KELVIN ATM 5.250000 2.260000 .303000-0

1 1 1	293.150000	-0.	27.430000	-0.
1 1 1	293.150000	-0.	48.640000	-0.
1 1 1	293.150000	-0.	63.410000	-0.
1 1 1	169.510000	-0.	21.440000	-0.
1 1 1	169.510000	-0.	49.960000	-0.
1 1 1	71.640000	-0.	20.100000	-0.
1 1 1	48.140000	-0.	55.060000	-0.
1 1 1	17.110000	-0.	22.500000	-0.
1 1 1	4.270000	-0.	.993000	-0.
1 1 1	3.460000	-0.	.570000	-0.
-0 1 1	2.620000	-0.	.064900	-0.

NC	T	P	TR	PR	ZK	ZEXP	ZCALC	DIFF
1	293.1500	27.4300	55.838	12.137	1.019	1.014	1.018	-.005
2	293.1500	48.6400	55.838	21.522	1.033	1.022	1.033	-.010
3	293.1500	63.4100	55.838	26.058	1.043	1.030	1.042	-.013
4	169.5100	21.4400	32.288	9.487	1.025	1.018	1.024	-.006
5	169.5100	49.9600	32.288	22.106	1.058	1.044	1.056	-.012
6	71.6400	20.1000	13.546	8.894	1.052	1.036	1.048	-.013
7	48.1400	55.0600	9.170	24.353	1.207	1.139	1.136	-.047
8	17.1100	22.5000	3.759	9.956	1.144	1.001	1.102	-.101
9	4.2700	.9930	.913	.439	.594	.634	.620	.065

10	3.4600	.5700	.659	.252	.075	.634	.071	.614
11	2.6300	.6649	.531	.029	.044	.845	9.300	0.
					.932	.893	.931	-.033
					.006	.893	.005	.388

BEATTIE MOLES PER LITER		-021-0	-0.	-0.
XENDN	KELVIN ATM	289.800000	57.890000	.292600-0

1	1	1	289.800000	-0.	57.780000	-0.
1	1	1	289.800000	-0.	57.880000	-0.
1	1	1	289.800000	-0.	57.910000	-0.
1	1	1	289.800000	-0.	58.020000	-0.
1	1	1	298.150000	-0.	65.970000	-0.
1	1	1	298.150000	-0.	67.320000	-0.
1	1	1	298.150000	-0.	68.600000	-0.
1	1	1	298.150000	-0.	70.380000	-0.
1	1	1	323.150000	-0.	89.320000	-0.
1	1	1	323.150000	-0.	95.580000	-0.
1	1	1	323.150000	-0.	101.690000	-0.
1	1	1	323.150000	-0.	109.390000	-0.
1	1	1	523.150000	-0.	275.570000	-0.
1	1	1	523.150000	-0.	321.390000	-0.
1	1	1	523.150000	-0.	372.920000	-0.
1	1	1	548.150000	-0.	298.510000	-0.
1	1	1	548.150000	-0.	349.180000	-0.
1	1	1	548.150000	-0.	406.150000	-0.
1	1	1	573.150000	-0.	321.160000	-0.
-0	1	1	573.150000	-0.	377.980000	-0.

NC	T	P	TR	PR	ZK	ZEXP	ZCALC	DIFF
1	289.8000	57.7800	1.000	.998	.361	.347	.346	.001
2	289.8000	57.8800	1.000	1.000	.299	.294	.315	-.011
3	289.8000	57.9100	1.000	1.000	.296	.271	.273	-.002
4	289.8000	58.0200	1.000	1.002	.289	.244	.258	-.014
5	298.1500	65.9700	1.029	1.140	.401	.385	.364	.021
6	298.1500	67.3200	1.029	1.163	.370	.344	.334	.010
7	298.1500	68.6000	1.029	1.135	.347	.312	.314	-.002
8	298.1500	70.3800	1.029	1.218	.329	.288	.297	-.009
9	323.1500	89.3200	1.115	1.552	.526	.434	.486	-.002
10	323.1500	95.5800	1.115	1.651	.481	.451	.461	-.011
11	323.1500	101.6900	1.115	1.757	.464	.426	.445	-.014
12	323.1500	109.3900	1.115	1.890	.454	.413	.435	-.007
13	523.1500	275.5700	1.305	4.760	.925	.917	.926	-.009
14	523.1500	321.3900	1.305	5.552	.945	.936	.946	-.010
15	523.1500	372.9200	1.305	6.442	.975	.965	.976	-.010
16	548.1500	298.5100	1.391	5.157	.953	.943	.955	-.007
17	548.1500	349.1800	1.391	6.032	.976	.970	.979	-.007
18	548.1500	406.1500	1.391	7.016	1.009	1.003	1.012	-.009
19	573.1500	321.1600	1.978	5.548	.978	.976	.981	-.005
20	573.1500	377.9800	1.978	6.514	1.004	1.002	1.009	-.007

LANDOLT AND BOERNSTEIN AMAGAT -0.1-0 -0. -0.
 HYDROGEN KELVIN ATM 33.244000 12.797000 .305000-0

1	1	1	33.240000	-0.	12.963000	-0.		
1	1	1	33.240000	-0.	51.457000	-0.		
1	1	1	36.840000	-0.	17.910000	-0.		
1	1	1	36.840000	-0.	40.635000	-0.		
1	1	1	55.820000	-0.	34.242000	-0.		
1	1	1	55.820000	-0.	56.525000	-0.		
1	1	2	203.150000	-0.	200.000000	400.000000		
1	1	4	273.150000	-0.	100.000000	300.000000		
1	1	2	372.400000	-0.	400.000000	300.000000		
1	1	2	473.400000	-0.	300.000000	300.000000		
-0	1	2	572.900000	-0.	200.000000	400.000000		

NC	T	P	TR	PR	ZK	ZEXP	ZCALC	DIFF
1	33.2400	12.9630	1.000	1.013	.272	.357	.258	.099
2	33.2400	51.4570	1.000	4.021	.594	.604	.609	-.005
2	36.8400	17.9100	1.108	1.400	.542	.495	.524	-.029
4	36.8400	40.6350	1.108	3.175	.531	.500	.514	-.014
5	55.8200	34.2420	1.079	2.676	.878	.829	.859	-.030
6	55.8200	56.5250	1.079	4.417	.883	.804	.859	-.055
7	203.1500	200.0000	6.111	15.629	1.180	1.162	1.145	.017
8	203.1500	600.0000	6.111	46.886	1.609	1.554	1.511	.044
9	203.1500	1000.0000	6.111	78.143	2.056	1.943	1.901	.042
10	273.1500	100.0000	8.217	7.914	1.069	1.070	1.058	.011
11	273.1500	400.0000	8.217	31.257	1.298	1.284	1.257	.027
12	273.1500	700.0000	8.217	54.700	1.541	1.505	1.471	.035
13	273.1500	1000.0000	8.217	78.143	1.780	1.721	1.689	.022
14	372.4000	400.0000	11.202	31.257	1.224	1.218	1.201	.017
15	372.4000	700.0000	11.202	54.700	1.402	1.375	1.361	.014
16	372.4000	1000.0000	11.202	78.143	1.582	1.536	1.524	.012
17	473.4000	200.0000	14.240	23.443	1.134	1.129	1.122	.007
18	473.4000	600.0000	14.240	46.886	1.272	1.256	1.250	.007
19	473.4000	900.0000	14.240	70.329	1.413	1.381	1.380	.001
20	572.9000	200.0000	17.233	15.629	1.074	1.073	1.069	.004
21	572.9000	600.0000	17.233	46.886	1.227	1.211	1.211	.000
22	572.9000	1000.0000	17.233	78.143	1.382	1.342	1.355	-.015

BARTLETT AND BEATTIE GRAMS-PER CC -021-0 2.0160 -0.
 HYDROGEN K. KELVIN ATM 33.244000 12.797000 .303500-0

1	1	2	273.150000	-0.	100.000000	200.000000		
-0	1	2	273.150000	-0.	600.000000	400.000000		

NC	T	P	TR	PR	ZK	ZEXP	ZCALC	DIFF
1	273.1500	100.0000	8.217	7.814	1.069	1.071	1.060	.011
2	273.1500	300.0000	8.217	23.443	1.219	1.205	1.193	.012
3	273.1500	600.0000	8.217	46.886	1.459	1.424	1.408	.016
4	273.1500	1000.0000	8.217	78.143	1.789	1.713	1.705	.009

BEATTIE AND SMITH CC PER GRAM -023-0 28.0140 -0.
 NITROGEN KELVIN ATM 126.020000 33.490000 .291700-0

1	1	1	323.120000	-0.	106.130000	-0.		
1	1	1	323.120000	-0.	138.263000	-0.		
1	1	1	323.120000	-0.	200.153000	-0.		
1	1	1	373.150000	-0.	125.564000	-0.		
1	1	1	373.150000	-0.	164.401000	-0.		
1	1	1	373.150000	-0.	240.052000	-0.		
1	1	1	473.150000	-0.	163.911000	-0.		
1	1	1	473.150000	-0.	216.152000	-0.		
-0	1	1	473.150000	-0.	319.534000	-0.		

NC	T	P	TR	PR	ZK	ZEXP	ZCALC	DIFF
1	323.1200	106.1300	2.584	3.159	1.004	1.009	1.010	-.001
2	323.1200	138.2630	2.584	4.128	1.014	1.023	1.022	.000
3	323.1200	200.1530	2.584	5.977	1.045	1.057	1.056	.001
4	373.1500	125.5640	2.961	3.749	1.026	1.034	1.034	.000
5	373.1500	164.4010	2.961	4.909	1.043	1.053	1.052	.001
6	373.1500	240.0520	2.961	7.168	1.083	1.098	1.097	.001
7	473.1500	163.9110	3.755	4.894	1.054	1.064	1.062	.002
8	473.1500	216.1520	3.755	6.454	1.078	1.092	1.088	.004
9	473.1500	319.5340	3.755	9.541	1.131	1.153	1.146	.006

BARTLETT AND BEATTIE GRAM PER CC -021-0 28.0140 -0.
 NITROGEN KELVIN ATM 126.020000 33.490000 .291700-0

1	1	2	273.150000	-0.	50.000000	50.000000		
-0	1	5	273.150000	-0.	200.000000	200.000000		

NC	T	P	TR	PR	ZK	ZEXP	ZCALC	DIFF
1	273.1500	50.0000	2.168	1.493	.976	.983	.981	.002
2	273.1500	100.0000	2.168	2.936	.971	.983	.976	.007
3	273.1500	200.0000	2.168	5.972	1.013	1.032	1.023	.009

4	273.1500	400.0000	2.158	11.944	1.213	1.253	1.226	.027
5	273.1500	600.0000	2.158	17.915	1.457	1.520	1.471	.049
6	273.1500	800.0000	2.158	23.838	1.710	1.797	1.725	.073
7	273.1500	1000.0000	2.153	29.860	1.965	2.065	1.979	.085

MICHELS AMAGAT -0.2-0 -0. -0.
 OXYGEN KELVIN ATM 154.330000 49.713000 .292100-0

1	1	1	273.150000	-0.	22.429000	-0.
1	1	1	273.150000	-0.	40.014400	-0.
1	1	1	273.150000	-0.	66.464600	-0.
1	1	1	273.150000	-0.	80.703600	-0.
1	1	1	273.150000	-0.	98.417400	-0.
1	1	1	273.150000	-0.	119.466000	-0.
1	1	1	298.150000	-0.	24.619600	-0.
1	1	1	298.150000	-0.	44.140100	-0.
1	1	1	298.150000	-0.	73.370300	-0.
1	1	1	298.150000	-0.	90.048600	-0.
1	1	1	298.150000	-0.	110.353700	-0.
1	1	1	298.150000	-0.	134.776700	-0.
1	1	1	323.150000	-0.	26.812300	-0.
1	1	1	323.150000	-0.	48.256700	-0.
1	1	1	323.150000	-0.	81.262300	-0.
-0	1	1	323.150000	-0.	99.401200	-0.
-0	1	1	323.150000	-0.	122.320800	-0.

NC	T	P	TR	PR	ZK	ZEXP	ZCALC	DIFF
1	273.1500	22.4290	1.770	.451	.977	.930	.981	-.001
2	273.1500	40.0144	1.770	.805	.960	.955	.964	.000
3	273.1500	66.4646	1.770	1.337	.938	.944	.942	.003
4	273.1500	80.7036	1.770	1.623	.928	.935	.931	.004
5	273.1500	98.4174	1.770	1.930	.918	.925	.920	.005
6	273.1500	119.4660	1.770	2.403	.908	.915	.910	.005
7	298.1500	24.6196	1.932	.495	.932	.986	.987	-.001
8	298.1500	44.1401	1.932	.889	.970	.975	.975	.000
9	298.1500	73.3703	1.932	1.486	.955	.951	.959	.002
10	298.1500	90.0486	1.932	1.811	.949	.956	.952	.003
11	298.1500	110.3537	1.932	2.220	.942	.950	.946	.004
12	298.1500	134.7767	1.932	2.711	.938	.946	.941	.005
13	323.1500	26.8123	2.094	.539	.987	.990	.991	-.001
14	323.1500	48.2567	2.094	.971	.979	.983	.983	.000
15	323.1500	81.2623	2.094	1.635	.969	.976	.973	.003
16	323.1500	99.4012	2.094	2.000	.965	.973	.969	.004
17	323.1500	122.3208	2.094	2.461	.962	.972	.967	.005

2. The Program ES68M

2.1. General Scope

The Program ES68M can be used for the calculation of the compressibility factor, the enthalpy, the entropy and the fugacity coefficient for a pure substance, as well as the same mean quantities and the individual fugacity coefficients for a mixture (up to 10 components). Enthalpy and entropy can be computed.

The Program is written in Fortram IV. It consists of the main program ES68M and the subroutine VIETA.

The data cards to be introduced are:

- (1) the Title Card which states the title of the problem.

The integer KCL controls intermediate quantities to be printed out; KE controls the output options.

- (2) the Substance Card gives the name of the substance, the critical temperature TM critical pressure PM and critical compressibility factor ZM. For a mixture of NC components (where $NC \leq 10$), each substance card gives the name of one component, the critical temperature TC(J), pressure PC(J) and compressibility factor ZC(J).
- (3) the Interaction Coefficients for mixtures are optional for the calculation. The symmetric matrix WW is presented to the computer as the components $(WW_{jm} - 1)$ with $j = 2, 3, \dots, NC$ and $m = 2, 3, \dots, j-1$. One card is used for each value of j. If no interaction coefficients are introduced, (NC-1) blank cards must be inserted.
- (4) the composition card gives the mole fraction of each component in the mixtures. Omit this card for a pure substance. A positive value for KY means that another composition card will follow. KY = 0 means the last composition card of the problem.

- (5) the Temperature-Pressure Schedule Cards allow a variety of prescriptions for different sets of temperatures and pressures. The T-schedule provides for sets consisting of a starting temperature T_L and an arbitrary number (NOT-1) higher temperature $T_L + DT$, $T_L + 2DT$, $T_L + 3DT$,at equal intervals. The P-schedule also provides for sets consisting of a starting pressure DP and any number (NPO-1) of higher pressures $2DP$, $3DP$, $4DP$ at equal intervals. Several sets of T-P schedules may be put in provided the total number of points (sum of the products $NOP \cdot NOT \cdot NC$) does not exceed 99. Any positive value for KS in the schedule card means that another schedule card follows. The last schedule card carries $KS = 0$.

After the temperature-pressure schedule cards a new composition card can be inserted for the same components. New temperature-pressure cards must follow.

Calculation for a new substance (pure or mixed) can be prescribed simply by adding a new complete set starting with the Title card and so on. A card containing $KCL = -1$ will terminate the computation.

The data are to be given in arbitrary but consistent absolute units throughout, e.g., all temperatures in $^{\circ}K$, and pressures in atm, etc. The output is dimensionless.

For the various schedules, the following outputs are available:

- (1) only the pseudo-critical quantities T_M , P_M and Z_M ;
- (2) in addition, the compressibility factor Z ;
- (3) only T_M, P_M, Z_M and Z and the mean fugacity coefficient ϕ ;
- (4) in addition, the mean heat content function $4/RT$ and the mean entropy expressed as S/R ;

- (5) in addition to (3), the individual fugacity coefficients ϕ_i ;
- (6) all options combined.

These options are controlled by the control quantity KE.

The calculation of fugacities requires an integration with respect to the pressure; individual fugacity coefficients require differentiations with respect to the composition; the calculation of the terms H/RT and S/R requires a differentiation with respect to the temperature. The temperature interval ET and the composition interval EY should be chosen such that the difference of the function values for $T_r + ET$ or $Y_s + EY$ furnishes about four significant figures. Any input for ET and EY overrides the standard choices $EY = 0.0003$ and $ET = 0.0001$.

The number NS of pressure subdivisions for the integrations is to be chosen differently for various purposes. In general, a pressure interval $DP/NS = 0.1$ in reduced units will be satisfactory for fugacity coefficients. For supercritical temperatures larger intervals will be sufficient. Smaller intervals may be desirable for the computation of H and S. The choice will depend, of course, on the desired precision. The program allows values of NS up to 50. Restriction of NS is desirable for economy in computer time.

22. Input

1. Title Card

column

- 2-37 Title of the problem.
- 38-39 KCL = Print intermediate quantities:
0 no print
9 print
-1 termination
- 40-41 NC: number of components in mixture
NC = 1 for pure substances
NC \leq 10 for mixtures
- 42-43 NPC: Reserved for punch control
- 44-45 NS: number of subdivisions of DP desired in
the integration
- 46-47 LAA: maximum number of approximation cycles;
LAA = 0: computer sets LA = 30;
LAA > 0: computer sets number of
approximation cycle LA = LAA + 10.
- 48-49 KE: controls the output options
0 same as KE = 3
1 only the pseudo-critical values TM, PM, ZM
are computed
2 compressibility factor Z
3 (in addition) mean fugacity coefficient
4 (in addition) individual fugacity coefficients
5 (in addition to 3) H/RT, S/R
6 all options combined

50-59 (6 dec.) EY: alteration in the composition of mixtures
If EY = 0, computer automatically sets
EY = 0.0003.

.60-69 (6 dec.) ET: temperature interval
If ET = 0, computer sets ET = 0.0001.

2. Substance Card(s)

For a pure substance:

Column

2-24 name of the substance.
25-36 (6 dec.) TM: critical temperature in any absolute unit.
37-48 (6 dec.) PM: critical pressure in any absolute unit.
49-60 (6 dec.) ZM: critical compressibility factor.

For a mixture (NC cards, one for each component. $NC \leq 10$)

Column

2-24 Name of the component in the mixture.
25-36 (6 dec.) TC (J): critical temperature in any absolute
unit
37-48 (6 dec.) PC (J): critical pressure in any absolute
unit
49-60 (6 dec.) ZC (J): critical compressibility factor

3. Interaction Coefficient Card

Column

2-8 (4 dec.) WW (J,M) J = 2, 3,NC
9-15 (4 dec.) WW (J,M) M = 1, 2,J-1
16-22 (4 dec.) WW (J,M)

23-29 (4 dec.) WW (J,M)

30-36 (4 dec.) WW (J,M)

37-43 (4 dec.) WW (J,M)

44-50 (4 dec.) WW (J,M)

51-57 (4 dec.) WW (J,M)

58-64 (4 dec.) WW (J,M)

4. Composition Card

Column

2-3

KY: control

KY > 0 indicates that the composition card is to be followed (after the T-P-schedule card) by another composition card for the same components.

KY = 0 means that the composition card is the last in the set.

4-9 (4 dec.)

YS(M): M = 1, 2,NC

10-15 (4 dec.)

16-21 (4 dec.)

22-27 (4 dec.)

28-33 (4 dec.)

34-39 (4 dec.)

40-45 (4 dec.)

46-51 (4 dec.)

52-57 (4 dec.)

58-63 (4 dec.)

5. T-P Schedule Cards (to be inserted after each composition card)

Column

2-3	KS: control
	KS > 0 indicates that the schedule card is to be followed by another one.
	KS = 0 means that the schedule card is the last in the set.
4-5	NOT: number of temperatures to be introduced
6-7	NOP: number of pressures to be introduced.
8-19 (6 dec.)	TL: lowest temperature to be introduced, in the same unit as TC.
20-31 (6 dec.)	DT: temperature increment in the same unit as TC.
32-43 (6 dec.)	DP: lowest pressure to be introduced. If NOP > 1, DP also indicates the pressure increment in the same unit as PC.

6. A complete set of data cards starting with the Title Card may be put in for a new problem. A new count of points (up to 99) starts. A card containing KCL = -1 in col. 38-39 terminates the calculation.

23. Control Integers

KE

The integer KE controls the output of the program. It may be some number between 0 and 6.

<u>Number</u>	<u>Output</u>
0	The computer automatically sets KE = 3. Only the fugacity coefficient, TM, PM, ZM and Z are calculated.
1	The computer calculates only the pseudo-critical temperature TM, pressure PM and compressibility factor ZM of the mixture.
2	The computer calculates TM, PM, ZM and the compressibility factor Z.
3	Same as KE = 0
4	The computer calculates the above quantities, namely: TM, PM, ZM, Z, ϕ plus the individual fugacity coefficients ϕ_i .
5	The computer calculates TM, PM, ZM, ZF, ϕ plus H/RT, S/R. This is applicable for pure substances.
6	The computer calculates all the quantities mentioned: TM, PM, ZM, ZF, ϕ , ϕ_i , H and S.

KH

The integer KH is generated in the program for the computation of heat content and entropy.

<u>Number</u>	<u>Output</u>
0	No calculation of H and S is desired. For $KE \leq 4$, KH is set to 0.
1	Calculation of H and S is desired. For $KE = 5$ or 6, KH is set to 1.

KF

The integer KF is provided for the beginning and end of the alteration in the composition. (Repeat control for ϕ_i .)

KF = 1 : first alteration

KF = 0 : last alteration

KCL

A diagnostic option KCL is provided at the end of the approximation cycle. If KCL = 9 several intermediate quantities will be printed out.

<u>Format</u>	<u>Quantities</u>
19	ME: number of the point
	TRR: reduced temp.
	PRR: reduced pressure
	QZ: mixing factor for $T_r > 1.02$
	ZK: Z obtained by the equation of Redlich and Kwong.
	ZGG(ME): Z obtained by the modified eq.
	ZG(ME): Z obtained by mixing ZK and ZGG(ME).

Format

Quantities

ZF(ME): final Z obtained from ZG by addition of derivation function DC.

DC: deviation function for $T_r > 1.02$

UP: numerator of DC

42

ME

TRR

XC This and the following quantities are intermediates

XC in the computation of $\log \phi$

EX

FGG

FG

SE(MS)

FN(ME) $\log \phi_K$

FM(ME) $\log \phi$

42

ME

PRR

EA Intermediates

EB

EC

ED

EW

FD

SD(MS)

DC

<u>Format</u>	<u>Quantities</u>
37	MH = number of point
	TH(MH) = temperature (altered)
	PH(MH) = pressure (altered)
	FH(MH) = $\log \phi$ for TH(MH)
	FM(MH) = $\log \phi$ for basic temperature
	PLG = $\log P_r$
	MTP(MH) discriminator for the altered temperature, defined between addresses 309 and 313
	MTPH(MH) same for the basic temperature

24. Output

<u>Format</u>	<u>Quantities</u>
11	(Title Card): KCL, NC, NPC, NS, LAA, KE, EY, ET
13	(Substance Card): TM, PM, ZM for a pure substance TC(J), PC(J), ZC(J) for a mixture (Interaction coefficient Card): WW(J,M), M = 1, NC J = 2, NC
16	(Composition Card): KY, (YS(M), M = 1, NC)
17	TM: pseudo critical temp for a mixture PM: pseudo critical pressure for a mixture ZM: pseudo critical compressibility factor
15	(Temperature-Pressure Schedule Cards): KS, NOT, NOP, TL, DT, DP
18	ME: number of the point JA: number of the approximation cycle

Format

QUANTITIES

MTYPE: -1 three phases

0 critical

1 a single phase

A(M): factors of the cubic equation (input for
VIETA)

X(N): roots (output of VIETA)

(Format 18 is printed out only if the solution of
the modified cubic equation is not obtained within
0.0004 (in Z) after LAA approximation cycles).

20

ME

TK: absolute temperature

PA: absolute pressure

TRR: T_r

PRR: P_r

ZK: Z obtained from the eq. of Redlich and Kwong

ZF(ME): Z obtained from ES68

FKD: $\log \phi$ obtained from R-K equation

22

ME

TK: absolute T

PA: absolute P

TR(ME): T_r

PR(ME): P_r

FKD: $\log \phi_K$

FMD: $\log \phi$ from modified equation

FFK: ϕ_K

FFM: ϕ

Format

Quantities

23	MF: number of the point
	TH(MF): absolute T
	PH(MF): absolute P
	$FDW = \sum y_i \log \phi_i$ Kwong
	$FDY = \sum y_i \log \phi_i$
	$FWD(1) = \log \phi_{1K}$
	$FYD(1) = \log \phi_1$
	$FFW(1) = \phi_{1K}$
	$FFY(1) = \phi_1$
24	$FWD(JC) = \log \phi_{iK}$ (other than 1st & last)
	$FYD(JC) = \log \phi_i$ (other than 1st & last)
	$FFW(JC) = \phi_{iK}$ (other than 1st & last)
	$FFY(JC) = \phi_i$ (other than 1st & last)
25	$FWC(NC) = y_i \log \phi_{iK}$
	$FYC(NC) = y_i \log \phi_i$
	$FWD(NC) = \log \phi_K$ for last component
	$FYD(NC) = \log \phi$ for last component
	$FFW(NC) = \phi_{iK}$ for last component
	$FFY(NC) = \phi_i$ for last component
38	MH: number of the point
	TH(MH): absolute T
	PH(MH): absolute P
	TR(MH): T_r
	PR(MH): P_r
	HT: mean heat content H/RT
	SR: mean entropy S/R

25. Various Symbols

<u>Symbols</u>	<u>Equivalents</u>
DIT	P_r for left end of the interval
PS(JS)	P_r for point JS (defining end interval DP)
ZL(1)	Z_K for the 1st phase
ZL(Z)	Z_K for the 2nd phase
FL(JK)	ϕ_K for the 1st and 2nd phase
ZS(JS)	Z_K for the supposedly stable phase of VIETA
ZN(ME) = ZK	
FN(ME) = FK	
AV(ME) = AK(=A ² P)	
BV(ME) = BK(=BP)	Kwong values for storage
FV(ME) = FK	
ZGG(ME) = ZS(MS): Z of the selected phase for a main point (for storage)	
AU(ME,JC) = AR(JC)	A and B individual
BU(ME,JC) = BR(JC)	Kwong coeff. for storage
FKD = log ϕ_K	
F(DC)	Contribution of DC to log ϕ
XC	Argument of arc tan for F (DC)
EX, EW	intermediates in F (DC)
ZH(MF) = ZF(MF)	
FH(MF) = FN(MF) = FK	for storage in alterations
TMM = TM	
PMM = PM	

$$FX(MF,JC) = \frac{\partial \ln \phi(MF)}{\partial y(JC)}$$

$$FS = \sum y_a \frac{\partial \ln \phi}{\partial y_a} = \sum y_s(JC) \cdot FY(MF,JC)$$

$$AUX = Z_K - B_K P$$

$$FY(MF,JC) = \ln \phi_{JC}$$

$$FW(MF,JC) = \ln \phi_{JC, Kwong}$$

$$FYC = \sum y_j \ln \phi_j$$

$$FWC = \sum y_i \ln \phi_{jK}$$

26. Program and Examples

After the Main Program ES68M the program of the Subroutine VIETA must be inserted. It is identical with the subroutine used in ES68Z.

The sources for the examples are:

Sulfur dioxide: Kang et al. (1961)

Ethane: Sage and Lacey (1950)

N-butane-carbon dioxide: Sage and Lacey (1955).

```
PROGRAM ES68M(INPUT,OUTPUT)
CES68M EQUATION OF STATE (MIXTURES,FUG,ENTH,ENTROPY) 10 APRIL 1969
DIMENSION TI(6),SUB(10,4),TC(10),PC(10),ZC(10),KW(10,10),Y(3),
2AA(10),BA(10),TR(100),PR(100),A(4),E(4),PS(51),ES(51),
3YS(10),YV(3),ZL(2),FL(2),ZA(100),X(3),ZS(51),AR(10),BR(10),
4EL(51),SE(51),ZN(100),FN(100),ZGG(100),ZG(100),ZF(100),AU(100,10),
5BU(100,10),AV(100),RV(100),FV(100),FM(100),TH(100),PH(100),
6ZH(100),FH(100),FKH(100),FY(100,10),FW(100,10),MTP(100),MTPH(100),
7FWD(10),FYC(10),FYD(10),FWC(10),FFW(10),FFY(10),FX(100,10),
8,SD(51),DCP(51)
11 FORMAT (1X,6A6,6I2,2F10.6)
12 FORMAT (///)
13 FORMAT (1X,A5,3A6,3F12.6)
14 FORMAT (1X, 9F7.3)
15 FORMAT (1X,3I2,3F12.6)
16 FORMAT (1X,I2,10F6.4)
17 FORMAT (24X,3F12.6)
18 FORMAT (1X,3I3,7H VIETA ,6F9.4)
19 FORMAT (2H D,I2,8F6.3,F12.4)
20 FORMAT (1X,I3,2F10.3,2F7.3,F8.3,F10.3,F10.4)
22 FORMAT (1X,I3,2F10.3,2F7.3,2F9.4,2F8.3)
23 FORMAT (1X,I3,2F10.3,4F8.4,2F8.3)
24 FORMAT (40X,2F8.4,2F8.3)
25 FORMAT (24X,4F9.4,2F8.3)
26 FORMAT (54H
27 FORMAT (69H NO T P TR PR PM ZM)
LOG FK )
ZK ZF
28 FORMAT (69H NO T P TR PR LOG FK LCG FM
2 FK FM )
29 FORMAT (69H NO T P LOG FWW LCG FYY LOG FW LOG FY
2 FW FY )
31 FORMAT (1H1,6A6,6I2,2F10.6)
32 FORMAT (1X,2I2,6F11.4)
33 FORMAT(1X, I3, 5F10.4, I3)
34 FORMAT (I5)
35 FORMAT (1X,6F11.6,I3)
36 FORMAT (57H NO T P TR PR HT
2SR)
37 FORMAT (2H D,I2,2F10.4,3F8.5,2I4 )
38 FORMAT(1X,I3,2F10.3,2F7.3,2F11.4)
39 FORMAT (1X,14HMOLE FRACTIONS )
40 FORMAT (1X,42H H P TL DT DP )
41 FORMAT (1X,I2,I3,11F6.3)
42 FORMAT (2H D,I2,2F6.3,7F8.4)
```

```
C
C INPUT AND PREPARATION
READ 11,(TI(M),M=1,6),KCL,NC,NPC,NS,LAA,KE,EY,ET
101 PRINT 31,(TI(M),M=1,6),KCL,NC,NPC,NS,LAA,KE,EY,ET
IF (NS.EQ. 0) NS=1
IF (KE) 81,82,81
82 KE=3
81 KH=0
IF (KE-4) 84,84,83
83 KH=1
84 CONTINUE
85 IF (EY) 88,89,88
89 EY=0.0003
88 IF (ET) 90,91,90
91 ET=0.0001
90 CONTINUE
IF (NC-1) 102,102,103
```

CES68M EQUATION OF STATE (MIXTURES, FUG, ENTH, ENTROPY) 16 FEBRUARY 1970

PROGRAM ES68M(INPUT,OUTPUT)

```

DIMENSION TI(6),SUB(10,4),TC(10),PC(10),ZC(10),WW(10,10),Y(3),
2AA(10),BA(10),TR(100),PR(100),A(4),E(4),PS(51),ES(51),
3YS(10),YV(3),ZC(2),FL(2),ZA(100),X(3),ZS(51),AR(10),BR(10),
4EL(51),SE(51),ZN(100),FN(100),ZGG(100),ZG(100),ZF(100),AU(100,10),
5BU(100,10),AV(100),BV(100),FV(100),FM(100),TH(100),PH(100),
6ZH(100),FH(100),FKH(100),FY(100,10),FW(100,10),MTP(100),MTPH(100),
7FWU(10),FYC(10),FYU(10),FWC(10),FFW(10),FFY(10),FX(100,10)
8,SD(51),DCP(51),DPP(100)

```

```

11 FORMAT (1X,6A6,6I2,2F10,6)
12 FORMAT (///)
13 FORMAT (1X,A5,3A6,3F12,6)
14 FORMAT (1X,9F7,3)
15 FORMAT (1X,3I2,3F12,6)
16 FORMAT (1X,I2,10F6,4)
17 FORMAT (24X,3F12,6)
18 FORMAT (1X,3I3,7H VIETA ,6F9,4)
19 FORMAT (2H 0,I2,8F6,3,F12,4)
20 FORMAT (1X,I3,2F10,3,2F7,3,F8,3,F10,3,F10,4)
22 FORMAT (1X,I3,2F10,3,2F7,3,2F9,4,2F8,3)
23 FORMAT (1X,I3,2F10,3,4F8,4,2F8,3)
24 FORMAT (40X,2F8,4,2F8,3)
25 FORMAT (24X,4F8,4,2F8,3)
26 FORMAT (54H
27 FORMAT (69H NO I P TR PR PM ZM
ZK ZF
2 LOG FK )
28 FORMAT (69H NO I P TR PR LOG FK LOG FM
2 FK FM )
29 FORMAT (69H NO I P LOG FWW LOG FYY LOG FW LOG FY
2 FW FY )
31 FORMAT (1H1,6A6,6I2,2F10,6)
32 FORMAT (1X,2I2,6F11,4)
33 FORMAT (1X, I3, 5F10,4, I3)
34 FORMAT (I5)
35 FORMAT (1X,6F11,6,I3)
36 FORMAT (57H NO I P TR PR HT
2SR)
37 FORMAT (2H 0,I2,2F10,4,3F8,5,2I4 )
38 FORMAT (1X,I3,2F10,3,2F7,3,2F11,4)
39 FORMAT (1X,14HMOLE FRACTIONS )
40 FORMAT (1X,42H H P TL DT DP )
41 FORMAT (1X,I2,I3,11F6,3)
42 FORMAT (2H 0,I2,2F6,3,7F8,4)
43 FORMAT (1X,I2,2F7,3,26H BEYOND RANGE OF R AND K )
44 FORMAT (1X,I2,2F7,3,17H NO CONVERGENCE )

```

C
C

INPUT AND PREPARATION

```

READ 11,(TI(M),M=1,6),KCL,NC,NPC,NS,LAA,KE,EY,ET
101 PRINT 31,(TI(M),M=1,6),KCL,NC,NPC,NS,LAA,KE,EY,ET
IF (NS.EQ.0) NS=1
IF (KE) 81,82,81
82 KE=3
81 KH=0
IF (KE=4) 84,84,83
83 KH=1
84 CONTINUE

```

```

85 IF (EY) 88,89,88
89 EY=0.0003
88 IF (ET) 90,91,90
91 ET=0.0001
90 CONTINUE
  IF (NC-1) 102,102,103
102 NC=1
  READ 13,(SUB(1,M),M=1,4),TM,PM,ZM
  PRINT 13,(SUB(1,M),M=1,4),TM,PM,ZM
  AM=3.847322*ZM*ZM*TM*TM*SQRT(TM)/PM
  BM=0.2599211*ZM*TM/PM
  GO TO 104
103 DO 105 J=1,NC
  READ 13,(SUB(J,M),M=1,4),TC(J),PC(J),ZC(J)
  AA(J)=3.847322*ZC(J)*ZC(J)*TC(J)*TC(J)*SQRT(TC(J))/PC(J)
  BA(J)=0.2599211*ZC(J)*TC(J)/PC(J)
105 PRINT 13,(SUB(J,M),M=1,4),TC(J),PC(J),ZC(J)
  DO 106 J=2,NC
  READ 14,(WW(J,M),M=1,NC)
  PRINT 14,(WW(J,M),M=1,NC)
106 CONTINUE
  DO 107 M=1,NC
  WW(M,M)=0.0
107 WW(1,M)=WW(M,1)

```

COMBINATION

```

108 READ 16,KY,(YS(M),M=1,NC)
  PRINT 12
  PRINT 39
  PRINT 16,KY,(YS(M),M=1,NC)
  KF=0
107 ZM=0.0
  BM=0.0
  AN=0.0
  AP=0.0
  PRINT 12
  DO 109 J=1,NC
  ZM=ZM+YS(J)*ZC(J)
  BM=BM+BA(J)*YS(J)
  SS=0.0
  DO 111 K=1,NC
111 SS=YS(K)*WW(J,K)*SQRT(AA(J)*AA(K))+SS
  AP=AP+YS(J)*SQRT(AA(J))
109 AN=AN+SS*YS(J)
  AM=AP*AP+AN
  IM=(0.2599211*0.2599211*AM/(ZM*BM))**0.6666667
  PM=TM*0.2599211*ZM/BM
  IF (KF.EQ.1) GO TO 104
  PRINT 26
  PRINT 17,TM,PM,ZM
104 IF (KE-1) 121,97,130

```

TEMPERATURE PRESSURE SCHEDULE

```

120 IF (KF-1) 121,122,122
122 DO 123 ME=1,MX
  TR(ME)=TR(ME)*IMM/TM
  DPP(ME)=DPP(ME)*PMM/PM
123 PR(ME)=PR(ME)*PMM/PM

```

```

GO TO 124
121 ME=0
PRINT 12
PRINT 40
113 READ 15,KS,NOT,NOP,TL,DT,DP
IF (KF.EQ.1) GO TO 110
PRINT 15,KS,NOT,NOP,TL,DT,DP
110 ME=ME+1
TR(ME)=TL/TM
127 IF (TR(ME)-0.722) 125,125,126
125 TR(ME)=TR(ME)+DT/TM
NOT=NOT-1
IF (NOT) 128,128,127
128 ME=ME-1
IF (KS) 129,129,113
129 IF (ME-1) 97,97,126
126 DO 114 JT=1,NOT
IF (JT-1) 115,116,115
115 ME=ME+1
TR(ME)=TR(ME-1)+DT/TM
116 PR(ME)=DP/PM
DPP(ME)=PR(ME)
IF(NOP.LT.2) GO TO 114
DO 117 JP=2,NOP
ME=ME+1
TR(ME)=TR(ME-1)
DPP(ME)=DPP(ME-1)
117 PR(ME)=PR(ME-1)+DP/PM
114 CONTINUE
IF (KS) 113,118,113
118 MX=ME
124 IF (LAA) 119,119,120
119 LAA=30
120 LA=LAA+10
A(1)=1.0
E(1)=1.0
E(2)=-1.0
IF (KF.EQ.1) GO TO 504
PRINT 12
PRINT 27
ANS=FLOAT(NS)

```

C
C

```

MAIN CYCLE
504 MS=NS+1
DO 201 ME=1,MX
PRD=2.0*PR(ME)
IF (DPP(ME).GT.PRD) GO TO 240
DDP=DPP(ME)/ANS
DDD=1.001*DPP(ME)
IF (PR(ME).GT.DDD) GO TO 203
202 QIN=1.0
TRR=TR(ME)
TRS=SQRT(TRR)
TU=TRR-1.0
TI=TRR*TRR*TRR
QZ=1.0
IF (TRR-1.02) 215,215,216
216 QZ=1.0-EXP(-0.05/TU)

```

```

DCP(1)=0.0
SD(1)=0.0
215 CONTINUE
AB=3.847322*ZM*ZM/(TRH*TRR*TRS)
BB=0.2599211*ZM/TRR
DEN=(1.0+0.1*TRR)*(1.0+0.1*TRR)
W=0.1/(1.0+2.06*TU)
V=1.15*(1.0+2.26*TU)/DEN
U=0.103*(1.0+3.59*TU)/DEN
WA=EXP(2.30259*(1.0-3.0*ZM)/W)-1.0
PS(1)=0.0
ES(1)=0.0
EL(1)=0.0
SE(1)=0.0
GO TO 204

```

```

203 PS(1)=PR(ME-1)
ES(1)=ES(MS)
EL(1)=EL(MS)
SE(1)=SE(MS)
DCP(1)=DCP(MS)
SD(1)=SD(MS)

```

```

204 CONTINUE
DO 205 JS=2,MS
PRR=PS(JS-1)+DDP
PS(JS)=PRR

```

C
C

```

R AND K
IF (NC-1) 230,230,231
230 AK=0.4278*PRR/(TRR*TRH*TRS)
AR(1)=AK
BK=0.08667*PRR/TRR
BR(1)=BK
GO TO 233

```

```

231 BK=0.0
AQ=0.0
DO 232 JE=1,NC
TJ=TRR*TM/TC(JE)
TJS=SQRT(TJ)
PJ=PRR*PM/PC(JE)
AS=0.4278*PJ/(TJ*TJ*TJS)
AR(JE)=SQRT(AS)
AQ=AQ+YS(JE)*AR(JE)
BR(JE)=0.08667*PJ/TJ
BK=BK+YS(JE)*BR(JE)

```

```

232 CONTINUE
AK=AQ*AQ

```

```

233 CONTINUE
E(3)=AK-BK*(1.0+BK)
E(4)=-AK*BK
CALL VIETA(E,YV,MT)
IF (MT) 206,207,207

```

```

206 ZL(1)=YV(1)
ZL(2)=YV(3)
LK=2
GO TO 208

```

```

207 ZL(1)=YV(1)
LK=1

```

```

208 DO 209 JK=1,LK

```

```

DSS=ZL(JK)-BK
IF (DSS.GT.0.0) GO TO 209
PRINT 43,ME,TR(ME),PR(ME)
GO TO 240
209 FL(JK)=ZL(JK)-1.0-ALOG(ZL(JK)-BK)-AK*ALOG(1.0+BK/ZL(JK))/BK
IF (LK-1) 210,210,211
211 IF (FL(2)-FL(1)) 212,210,210
212 FK=FL(2)
ZK=ZL(2)
MP=2
GO TO 214
210 FK=FL(1)
ZK=ZL(1)
MP=1
214 CONTINUE
IF (FK.GT.100.0) GO TO 99
ZA(1)=ZK
AC=AB*PRR
BC=BB*PRR

```

APPROXIMATION CYCLE

```

DO 301 JA=1,LA
D=PRR*ZM/(TRR*ZA(JA))
S=D*(3.0-D*(3.0-D))
GLL=1.0+WA*S
GL=W*ALOG10(GLL)
IF (S-1.0) 306,307,307
306 WB=1.43/(TRR*IRS)-1.32
GL=GL*(WB+(1.0-WB)*S)
307 GLG=1.0+U*S*S*(S-1.0)*(S-1.0)
IF (GLG) 97,97,309
309 GG=V*ALOG10(GLG)
A(2)=GL-1.0
A(3)=AC*(1.0-GG)-BC*(1.0-GL+BC)
A(4)=-AC*BC*(1.0-GG)
CALL VIETA(A,X,MTYPE)
MTP(ME)=10*MTYPE+MP
IF (JA=LAA) 312,312,313
313 PRINT 18,ME,JA,MTYPE,(A(M),M=2,4),(X(N),N=1,3)
312 IF (MTYPE) 314,315,315
314 IF (MP-1) 315,315,316
316 ZS(JS)=X(3)
GO TO 317
315 ZS(JS)=X(1)
317 IF (ABS(ZS(JS)-ZA(JA))-0.0004) 318,319,319
319 IF (JA-10) 320,320,321
321 DIS=(ZS(JS)-ZA(JA))*(ZA(JA)-ZA(JA-1))
IF (DIS) 322,322,323
322 QIN=0.9*QIN
GO TO 320
323 QIN=1.05*QIN
IF (QIN-1.0) 320,320,324
324 QIN=1.0
320 ZA(JA+1)=QIN*ZS(JS)+(1.0-QIN)*ZA(JA)
301 CONTINUE
PRINT 44,ME,TR(ME),PR(ME)
240 DPP(ME)=10.0*PR(ME)
IF (ME.EQ.MX) GO TO 201

```

```

IF (TR(ME+1).EQ.TR(ME)) DPP(ME+1)=DPP(ME)
GO TO 201
318 ES(JS)=AC*GG/(ZS(JS)+BC)-ZS(JS)*GL/(ZS(JS)-BC)
ES(JS)=ES(JS)+ZS(JS)/PRR
EL(JS)=PRR/ZS(JS)
IF (EL(JS-1).NE.0.0) GO TO 325
ES(JS-1)=ES(JS)
325 SE(JS)=SE(JS-1)+0.5*(ES(JS)+ES(JS-1))*(EL(JS)-EL(JS-1))
IF (TRR-1.02) 326,326,327
327 UP=(3.281-11.10*ZM)*(TT-2.6*TU+((4.36-15.0*ZM)*TRR-6.70+21.3*ZM)*
2SQRT(PRR))
DCP(JS)=UP*TU/(TT*TT+0.4*PRR*PRR)
SD(JS)=SD(JS-1)+0.5*(DCP(JS-1)+DCP(JS))*DDP
GO TO 328
326 SD(JS)=0.0
DCP(JS)=0.0
328 CONTINUE
305 CONTINUE
ZN(ME)=ZK
FN(ME)=FK
ZGG(ME)=ZS(MS)
ZG(ME)=ZGG(ME)
DC=0.0
UP=0.0
IF (TRR-1.02) 217,217,218
218 ZG(ME)=ZK+QZ*(ZGG(ME)-ZK)
UP=(3.281-11.10*ZM)*(TT-2.6*TU+((4.36-15.0*ZM)*TRR-6.70+21.3*ZM)*
2SQRT(PRR))
DC=UP*TU*PRR/(TT*TT+0.4*PRR*PRR)
217 ZF(ME)=ZG(ME)+DC
DO 234 JD=1,NC
AU(ME,JD)=AR(JD)*AR(JD)
234 BU(ME,JD)=BR(JD)
AV(ME)=AK
BV(ME)=BK
FV(ME)=FK
FKD=0.434294*FK
IF (KCL-9) 219,220,219
220 PRINT 19,ME,TRR,PRR,QZ,ZK,ZGG(ME),ZG(ME),ZF(ME),DC,UP
219 IK=TRR*TM
PA=PRR*PM
IF (KF.EQ.1) GO TO 236
IF (KH.EQ.2) GO TO 236
PRINT 20,ME,IK,PA,TRR,PRR,ZK,ZF(ME),FKD
236 IF (KE-2) 221,201,221
C
C
FUGACITY COEFFICIENT
221 FGG=ZGG(ME)-1.0-ALOG(ZGG(ME)-BC)-AC*ALOG(1.0+BC/ZGG(ME))/BC+SE(MS)
FG=FGG
FD=0.0
EA=0.0
EB=0.0
EC=0.0
ED=0.0
EW=0.0
EX=0.0
XC=0.0
YC=0.0

```

```

IF (TRR-1.52) 222,222,223
223 EA=(3.281-11.10*ZM)*(TT-2.6*TU)*TU/(TT*0.632456)
EB=(3.281-11.10*ZM)*((4.36-15.0*ZM)*TRR-6.70+21.3*ZM)*TU/(TT*TT)
EC=SQRT(0.632456/TT)
XC=EC*EC*PRR
YC=EC*SQRT(PRR)
EX=ATAN(XC)
IF (ABS(XC-1.0)-0.0001) 238,238,237
238 EU=1.5707963
GO TO 239
237 EU=ATAN(1.414213*YC/(1-XC))
IF (XC.LT.1.0) GO TO 239
ED=1.1415926+ED
239 EW=0.176777*ALOG((1.0-1.414213*YC+YC*YC)/(1.0+1.414213*YC+YC*YC))+
20.353554*ED
FD=EA*EX+2.0*EB*EW/(EC*EC*EC)
FG=FN(ME)+QZ*(FGG-FN(ME))
222 FM(ME)=FG+FD
IF (KCL-9) 201,224,201
224 PRINT 12
PRINT 42,ME,TRR,XC,YC,EX,FGG,FG,SE(MS),FN(ME),FM(ME)
PRINT 42,ME,PRR,EA,EB,EC,ED,EW,FD,SD(MS),DC
PRINT 12
201 CONTINUE
IF (KE.LT.3) GO TO 97
IF (KF-1) 225,402,402
225 IF (KH-1) 226,226,502
226 PRINT 12
PRINT 28
DO 227 ME=1, MX
PRD=2.0*PR(ME)
IF (DPP(ME).GT.PRD) GO TO 227
TK=TR(ME)*TM
PA=PR(ME)*PM
FMD=0.434294*FM(ME)
FKD=0.434294*FN(ME)
FFK=EXP(FN(ME))
FFM=EXP(FM(ME))
PRINT 22,ME,TK,PA,TR(ME),PR(ME),FKD,FMD,FFK,FFM
227 CONTINUE
IF (KE-4) 97,228,228
228 DO 235 MF=1, MX
PRD=2.0*PR(MF)
IF (DPP(MF).GT.PRD) GO TO 235
TH(MF)=TR(MF)*TM
PH(MF)=PR(MF)*PM
ZH(MF)=ZF(MF)
FH(MF)=FM(MF)
MTPH(MF)=MTP(MF)
FKH(MF)=FN(MF)
235 CONTINUE
TMM=TM
PMM=PM
ZMM=ZM
IF (NC.EQ.1) GO TO 501
IF (KE-5) 401,501,401

```

INDIVIDUAL FUGACITY COEFFICIENTS

```

401 DO 404 JC=1,NC
    KF=1
    IF (YS(JC)-0.9) 405,405,406
406 EY=-EY
405 YS(JC)=YS(JC)+EY
    GO TO 407
402 DO 408 MF=1,MX
    PRD=2.0*PR(MF)
    IF (DPP(MF).GT.PRD) GO TO 408
    TR(MF)=TR(MF)*TM/TMM
    DPP(MF)=DPP(MF)*PM/PMM
    PR(MF)=PR(MF)*PM/PMM
    FX(MF,JC)=(FM(MF)-FH(MF))/EY
408 CONTINUE
    YS(JC)=YS(JC)-EY
    TM=TMM
    PM=PMM
    ZM=ZMM
    IF (YS(JC)-0.9) 404,404,416
416 EY=-EY
404 CONTINUE
    PRINT 12
    PRINT 29
    DO 409 MF=1,MX
    PRD=2.0*PR(MF)
    IF (DPP(MF).GT.PRD) GO TO 409
    FS=0.0
    DO 410 JC=1,NC
410 FS=FS+YS(JC)*FX(MF,JC)
    AUX=ALOG(ZN(MF)-BV(MF))
    FYY(MF)=0.0
    FWW(MF)=0.0
    DO 411 JC=1,NC
    FY(MF,JC)=FH(MF)+FX(MF,JC)-FS
    FW(MF,JC)=(ZN(MF)-1.0)*BU(MF,JC)/BV(MF)-AUX-
    2(AV(MF)/BV(MF))*(2.0*SQRT(AU(MF,JC)/AV(MF))-BU(MF,JC)/BV(MF))*
    3ALOG(1.0+BV(MF)/ZN(MF))
411 CONTINUE
409 CONTINUE
    DO 412 MF=1,MX
    PRD=2.0*PR(MF)
    IF (DPP(MF).GT.PRD) GO TO 412
    FDW=0.434294*FKH(MF)
    FDY=0.434294*FH(MF)
    FW(1)=0.434294*FW(MF,1)
    FY(1)=0.434294*FY(MF,1)
    FFW(1)=EXP(FW(MF,1))
    FFY(1)=EXP(FY(MF,1))
    PRINT 23,MF,TH(MF),PH(MF),FDW,FDY,FW(1),FY(1),FFW(1),FFY(1)
    ND=NC-1
    FWC(1)=YS(1)*FW(1)
    FYC(1)=YS(1)*FY(1)
    IF (NC-2) 413,413,414
414 DO 415 JC=2,ND
    FWD(JC)=0.434294*FW(MF,JC)
    FYD(JC)=0.434294*FY(MF,JC)
    FWC(JC)=FWC(JC-1)+YS(JC)*FWD(JC)
    FYC(JC)=FYC(JC-1)+YS(JC)*FYD(JC)

```

```

FFW(JC)=EXP(FW(MF,JC))
FFY(JC)=EXP(FY(MF,JC))
415 PRINT 24,FWD(JC),FYD(JC),FFW(JC),FFY(JC)
413 FWD(NC)=0.434294*FW(MF,NC)
FYD(NC)=0.434294*FY(MF,NC)
FWC(NC)=FWC(ND)+YS(NC)*FWD(NC)
FYC(NC)=FYC(ND)+YS(NC)*FYD(NC)
FFY(NC)=EXP(FY(MF,NC))
FFW(NC)=EXP(FW(MF,NC))
PRINT 25,FWC(NC),FYC(NC),FWD(NC),FYD(NC),FFW(NC),FFY(NC)
412 CONTINUE
KF=0
IF (KH-1) 97,501,97

HEAT CONTENT, ENTROPY
501 KH=2
PRINT 12
PRINT 36
DO 503 MH=1, MX
503 TR(MH)=TR(MH)+ET
GO TO 504
502 DO 505 MH=1, MX
PRD=2.0*PR(MH)
IF (DPP(MH).GT.PR) GO TO 505
TR(MH)=TR(MH)-ET
HT=(FH(MH)-FM(MH))*TR(MH)/ET
SK=HT-FH(MH)-ALOG(PR(MH))
PLG=ALOG(PR(MH))
IF (KCL-9) 506,507,506
507 PRINT 37,MH,TR(MH),PH(MH),FH(MH),FM(MH),PLG,MTP(MH),MTPH(MH)
506 CONTINUE
PRINT 38,MH,TR(MH),PH(MH),TR(MH),PR(MH),HT,SK
505 CONTINUE
KH=1
97 CONTINUE
IF (KY) 98,98,108
98 HEAD 11,(TI(M),M=1,6),KCL,NC,NPC,NS,LAA,KE,EY,ET
IF (KCL) 99,101,101
99 STOP
END

```

```

SUBROUTINE VIETA (A, Y, MTYPE)
SOLUTION OF THE GENERAL CUBIC EQUATION      MOD 4
A(1)*Y**3+A(2)*Y**2+A(3)*Y+A(4)=0
WITHOUT CUBERTF, ASINF, ACOSF, FOR GENERAL USE
DIMENSION A(4), B(3), Y(3)
B(1) = A(2)/A(1)
B1OV3 = B(1)/3.0
B(2) = A(3)/A(1)
B(3) = A(4)/A(1)
ALF = B(2) - B(1)*B1OV3
BET = 2.0*B1OV3**3 - B(2)*B1OV3 + B(3)
BE1OV2 = BET/2.0
ALFOV3 = ALF/3.0
CUAOV3 = ALFOV3**3
SQBOV2 = BE1OV2**2
DEL = SQBOV2 + CUAOV3
IF (DEL) 40,20,30

```

C MTYPE=0 TWO ROOTS EQUAL

```

20 MTYPE = 0
   GAM = SQRTF(-ALFOV3)
   IF (BET) 22,22,21
21 Y(1) = -2.0*GAM -B10V3
   Y(2) = GAM - B10V3
   Y(3) = Y(2)
   GO TO 50
22 Y(1) = 2.0*GAM -B10V3
   Y(2) = -GAM -B10V3
   Y(3) = Y(2)
   GO TO 50

```

C MTYPE=1 TWO COMPLEX ROOTS

```

30 MTYPE = 1
   EPS = SQRTF(DEL)
   TAU = -BETOV2
   RCU=TAU+EPS
   SCU=TAU-EPS
   SIR=1.0
   SIS=1.0
   IF (RCU) 31,32,32
31 SIR=-1.0
32 IF (SCU) 33,34,34
33 SIS=-1.0
34 R=SIR*(SIR+RCU)**0.33333333
   S=SIS*(SIS+SCU)**0.33333333

```

C Y(1)=REAL ROOT, Y(2)=REAL PART AND Y(3)=IMAGINARY PART OF TWO COMPLEX ROOTS

```

Y(1) = R + S - B10V3
Y(2) = -(R+S)/2.0 - B10V3
Y(3) = 0.86602540*(R-S)
GO TO 50

```

C MTYPE=-1 THREE REAL ROOTS

```

40 MTYPE = -1
   QUOT = SQBOV2/CUAOV3
   ROOT = SQRTF(-QUOT)
   IF (BET) 42,41,41
41 PHI = (1.5707963 + ATANF(ROOT / SQRTF(1.0 - ROOT**2))) / 3.0
   GO TO 43
42 PHI = ATANF(SQRTF(1.0 - ROOT**2) / ROOT) / 3.0
43 FACT = 2.0*SQRTF(-ALFOV3)
   Y(1) = FACT*COSEF(PHI) - B10V3
   Y(2) = FACT*COSEF(PHI + 2.0943951) - B10V3
   Y(3) = FACT*COSEF(PHI + 4.1887902) - B10V3

```

C Y(1) HIGHEST ROOT, Y(3) LOWEST ROOT

```

YA=AMAX1(Y(1),Y(2),Y(3))
YC=AMIN1(Y(1),Y(2),Y(3))
YB=Y(1)+Y(2)+Y(3)-YA-YC
Y(1)=YA
Y(2)=YB
Y(3)=YC

```

```

50 RETURN
END

```

```
102 NC=1
   READ 13,(SUB(I,M),M=1,4),TM,PM,ZM
   PRINT 13,(SUB(I,M),M=1,4),TM,PM,ZM
   AM=3.847322*ZM*ZM*TM*TM*SQRT(TM)/PM
   BM=0.2599211*ZM*TM/PM
   GO TO 104
103 DO 105 J=1,NC
   READ 13,(SUB(J,M),M=1,4),TC(J),PC(J),ZC(J)
   AA(J)=3.847322*ZC(J)*ZC(J)*TC(J)*TC(J)*SQRT(TC(J))/PC(J)
   BA(J)=0.2599211*ZC(J)*TC(J)/PC(J)
105 PRINT 13,(SUB(J,M),M=1,4),TC(J),PC(J),ZC(J)
   DO 106 J=2,NC
   READ 14,(WW(J,M),M=1,NC)
   PRINT 14,(WW(J,M),M=1,NC)
106 CONTINUE
   DO 107 M=1,NC
   WW(M,M)=0.0
107 WW(1,M)=WW(M,1)
C
C   COMBINATION
108 READ 16,KY,(YS(M),M=1,NC)
   PRINT 12
   PRINT 39
   PRINT 16,KY,(YS(M),M=1,NC)
   KF=0
407 ZM=0.0
   BM=0.0
   AN=0.0
   AP=0.0
   PRINT 12
   DO 109 J=1,NC
   ZM=ZM+YS(J)*ZC(J)
   BM=BM+BA(J)*YS(J)
   SS=0.0
   DO 111 K=1,NC
111 SS=YS(K)*WW(J,K)*SQRT(AA(J)*AA(K))+SS
   AP=AP+YS(J)*SQRT(AA(J))
109 AN=AN+SS*YS(J)
   AM=AP*AP*AN
   TM=(0.2599211*0.2599211*AM/(ZM*BM))**0.6666667
   PM=TM*0.2599211*ZM/BM
   IF (KF.EQ.1) GO TO 104
   PRINT 26
   PRINT 17,TM,PM,ZM
104 IF (KE-1) 121,97,130
C
C   TEMPERATURE PRESSURE SCHEDULE
130 IF (KF-1) 121,122,122
122 DO 123 ME=1,MX
   TR(ME)=TR(ME)*TMM/TM
123 PR(ME)=PR(ME)*PMM/PM
   GO TO 124
121 ME=0
113 READ 15,KS,NOT,NOP,TL,DT,DP
   IF (KF.EQ.1) GO TO 110
   PRINT 12
   PRINT 40
   PRINT 15,KS,NOT,NOP,TL,DT,DP
110 ME=ME+1
   TR(ME)=TL/TM
127 IF (TR(ME)-0.722) 125,125,126
125 TR(ME)=TR(ME)+DT/TM
```

```
NOT=NOT-1
IF (NOT) 128,128,127
128 ME=ME-1
IF (KS) 129,129,113
129 IF (ME-1) 97,97,126
126 DO 114 JT=1,NOT
IF (JT-1) 115,116,115
115 ME=ME+1
TR(ME)=TR(ME-1)+DT/TM
116 PR(ME)=DP/PM
IF(NOP. LT. 2) GO TO 114
DO 117 JP=2,NOP
ME=ME+1
TR(ME)=TR(ME-1)
117 PR(ME)=PR(ME-1)+DP/PM
114 CONTINUE
IF (KS) 113,118,113
118 MX=ME
124 IF (LAA) 119,119,120
119 LAA=30
120 LA=LAA+10
A(1)=1.0
E(1)=1.0
E(2)=-1.0
IF (KF.EQ.1) GO TO 504
PRINT 12
PRINT 27
```

C

```
MAIN CYCLE
504 MS=MS+1
DO 201 ME=1, MX
DIT=ABS(PR(ME)--DP/PM)-0.02*DP/PM
ANS=FLOAT(NS)
DDP=DP/(PM*ANS)
IF (DIT) 202,202,203
202 QIN=1.0
TRR=TR(ME)
TRS=SQRT(TRR)
TU=TRR-1.0
TT=TRR*TRR*TRR
QZ=1.0
IF (TRR-1.02) 215,215,216
216 QZ=1.0-EXP(-0.05/TU)
DCP(1)=0.0
SD(1)=0.0
215 CONTINUE
AB=3.847322*ZM*ZM/(TRR*TRR*TRS)
BB=0.2599211*ZM/TRR
DEN=(1.0+0.1*TRR)*(1.0+0.1*TRR)
W=0.1/(1.0+2.06*TRR)
V=1.15*(1.0+2.26*TRR)/DEN
U=0.103*(1.0+3.59*TRR)/DEN
WA=EXP(2.30259*(1.0-3.0*ZM)/W)-1.0
PS(1)=0.0
ES(1)=0.0
EL(1)=0.0
SE(1)=0.0
GO TO 204
203 PS(1)=PR(ME-1)
ES(1)=ES(MS)
EL(1)=EL(MS)
SE(1)=SE(MS)
```

```
DCP(1)=DCP(MS)
SD(1)=SD(MS)
204 CONTINUE
DO 205 JS=2,MS
PRR=PS(JS-1)+DDP
PS(JS)=PRR
C
C R AND K
IF (NC-1) 230,230,231
230 AK=0.4278*PRR/(TRR*TRR*TRS)
AR(1)=AK
BK=0.08667*PRR/TRR
BR(1)=BK
GO TO 233
231 BK=0.0
AQ=0.0
DO 232 JE=1,NC
TJ=TRR*TM/TC(JE)
TJS=SQRT(TJ)
PJ=PRR*PM/PC(JE)
AS=0.4278*PJ/(TJ*TJ*TJS)
AR(JE)=SQRT(AS)
AQ=AQ+YS(JE)*AR(JE)
BR(JE)=0.0867*PJ/TJ
BK=BK+YS(JE)*BR(JE)
232 CONTINUE
AK=AQ*AQ
233 CONTINUE
E(3)=AK-BK*(1.0+BK)
E(4)=-AK*BK
CALL VIETA(E,YV,MT)
IF (MT) 206,207,207
206 ZL(1)=YV(1)
ZL(2)=YV(3)
LK=2
GO TO 208
207 ZL(1)=YV(1)
LK=1
208 DO 209 JK=1,LK
209 FL(JK)=ZL(JK)-1.0-ALOG(ZL(JK)-BK)-AK*ALOG(1.0+BK/ZL(JK))/BK
IF (LK-1) 210,210,211
211 IF (FL(2)-FL(1)) 212,210,210
212 FK=FL(2)
ZK=ZL(2)
MP=2
GO TO 214
210 FK=FL(1)
ZK=ZL(1)
MP=1
214 CONTINUE
IF (FK .GT. 100.0) GO TO 99
ZA(1)=ZK
AC=AB*PRR
BC=BB*PRR
C
C APPROXIMATION CYCLE
DO 301 JA=1,LA
D=PRR*ZM/(TRR*ZA(JA))
S=D*(3.0-D*(3.0-D))
GLL=1.0+W*A*S
GL=W*ALOG10(GLL)
IF (S-1.0) 306,307,307
```

```
306 WB=1.43/(TRR*TRS)-1.32
    GL=GL*(WB+(1.0-WB)*S)
307 GLG=1.0+U*S*S*(S-1.0)*(S-1.0)
    IF (GLG) 97,97,309
309 GG=V*ALOG10(GLG)
    A(2)=GL-1.0
    A(3)=AC*(1.0-GG)-BC*(1.0-GL+BC)
    A(4)=-AC*BC*(1.0-GG)
    CALL VIETA(A,X,MTYPE)
    MTP(ME)=10*MTYPE+MP
    IF (JA-LAA) 312,312,313
313 PRINT 18,ME,JA,MTYPE,(A(M),M=2,4),(X(N),N=1,3)
312 IF (MTYPE) 314,315,315
314 IF (MP-1) 315,315,316
316 ZS(JS)=X(3)
    GD TO 317
315 ZS(JS)=X(1)
317 IF (ABS(ZS(JS)-ZA(JA))-0.0004) 318,319,319
319 IF (JA-10) 320,320,321
321 DIS=(ZS(JS)-ZA(JA))*(ZA(JA)-ZA(JA-1))
    IF (DIS) 322,322,323
322 QIN=0.9*QIN
    GO TO 320
323 QIN=1.05*QIN
    IF (QIN-1.0) 320,320,324
324 QIN=1.0
320 ZA(JA+1)=QIN*ZS(JS)+(1.0-QIN)*ZA(JA)
301 CONTINUE
    GO TO 97
318 ES(JS)=AC*GG/(ZS(JS)+BC)-ZS(JS)*GL/(ZS(JS)-BC)
    ES(JS)=ES(JS)*ZS(JS)/PRR
    EL(JS)=PRR/ZS(JS)
    IF (EL(JS-1).NE.0.0) GO TO 325
    ES(JS-1)=ES(JS)
325 SE(JS)=SE(JS-1)+0.5*(ES(JS)+ES(JS-1))*(EL(JS)-EL(JS-1))
    IF (TRR-1.02) 326,326,327
327 UP=(3.281-11.10*ZM)*(TT-2.6* $TU$ +(4.36-15.0*ZM)*TRR-6.70+21.3*ZM)*
    2SQRT(PRR)
    DCP(JS)=UP* $TU$ /(TT*TT+0.4*PRR*PRR)
    SD(JS)=SD(JS-1)+0.5*(DCP(JS-1)+DCP(JS))*DDP
    GO TO 323
326 SD(JS)=0.0
    DCP(JS)=0.0
328 CONTINUE
205 CONTINUE
    ZN(ME)=ZK
    FN(ME)=FK
    ZGG(ME)=ZS(MS)
    ZG(ME)=ZGG(ME)
    DC=0.0
    UP=0.0
    IF (TRR-1.02) 217,217,218
218 ZG(ME)=ZK+QZ*(ZGG(ME)-ZK)
    UP=(3.281-11.10*ZM)*(TT-2.6* $TU$ +(4.36-15.0*ZM)*TRR-6.70+21.3*ZM)*
    2SQRT(PRR)
    DC=UP* $TU$ *PRR/(TT*TT+0.4*PRR*PRR)
217 ZF(ME)=ZG(ME)+DC
    DO 234 JD=1,NC
    AU(ME,JD)=AR(JD)*AR(JD)
234 BU(ME,JD)=BR(JD)
    AV(ME)=AK
    BV(ME)=BK
```

```
FV(ME)=FK
FKD=0.434294*FK
IF (KCL-9) 219,220,219
220 PRINT 19,ME,TRR,PRR,QZ,ZK,ZGG(ME),ZG(ME),ZF(ME),DC,UP
219 TK=TRR*TM
PA=PRR*PM
IF (KF.EQ.1) GO TO 236
IF (KH.EQ.2) GO TO 236
PRINT 20,ME,TK,PA,TRR,PRR,ZK,ZF(ME),FKD
236 IF (KE-2) 221,201,221
C
C FUGACITY COEFFICIENT
221 FGG=ZGG(ME)-1.0-ALOG(ZGG(ME)-BC)-AC*ALOG(1.0+BC/ZGG(ME))/BC+SE(MS)
FG=FGG
FD=0.0
EA=0.0
EB=0.0
EC=0.0
ED=0.0
EW=0.0
EX=0.0
XC=0.0
YC=0.0
IF (TRR-1.02) 222,222,223
223 EA=(3.281-11.10*ZM)*(TT-2.6*TM)*TU/(TT*0.632456)
EB=(3.281-11.10*ZM)*((4.36-15.0*ZM)*TRR-6.70+21.3*ZM)*TU/(TT*TT)
EC=SQRT(0.632456/TT)
XC=EC*EC*PRR
YC=EC*SQRT(PRR)
EX=ATAN(XC)
IF (ABS(XC-1.0)-0.0001) 238,238,237
238 ED=1.5707963
GO TO 239
237 ED=ATAN(1.414213*YC/(1-XC))
IF (XC.LT.1.0) GO TO 239
ED=3.1415926+ED
239 EW=0.176777*ALOG((1.0-1.414213*YC+YC*YC)/(1.0+1.414213*YC+YC*YC))+
20.353554*ED
FD=EA*EX+2.0*EB*EW/(EC*EC*EC)
FG=FN(ME)+QZ*(FGG-FN(ME))
222 FM(ME)=FG+FD
IF (KCL-9) 201,224,201
224 PRINT 12
PRINT 42,ME,TRR,XC,YC,EX,FGG,FG,SE(MS),FN(ME),FM(ME)
PRINT 42,ME,PRR,EA,EB,EC,ED,EW,FD,SD(MS),DC
PRINT 12
201 CONTINUE
IF (KE.LT.3) GO TO 97
IF (KF-1) 225,402,402
225 IF (KH-1) 226,226,502
226 PRINT 12
PRINT 28
DO 227 ME=1,MX
TK=TR(ME)*TM
PA=PR(ME)*PM
FMD=0.434294*FM(ME)
FKD=0.434294*FN(ME)
FFK=EXP(FN(ME))
FFM=EXP(FM(ME))
227 PRINT 22,ME,TK,PA,TR(ME),PR(ME),FKD,FMD,FFK,FFM
IF (KE-4) 97,228,228
228 DO 235 MF=1,MX
```

```
TH(MF)=TR(MF)*TM
PH(MF)=PR(MF)*PM
ZH(MF)=ZF(MF)
FH(MF)=FM(MF)
MTPH(MF)=MTP(MF)
235 FKH(MF)=FN(MF)
TMM=TM
PMM=PM
ZMM=ZM
IF (NC .EQ. 1) GO TO 501
IF (KE-5) 401,501,401

C
C INDIVIDUAL FUGACITY COEFFICIENTS
401 DO 404 JC=1,NC
KF=1
IF (YS(JC)-0.9) 405,405,406
406 EY=-EY
405 YS(JC)=YS(JC)+EY
GO TO 407
402 DO 408 MF=1,MX
TR(MF)=TR(MF)*TM/TMM
PR(MF)=PR(MF)*PM/PMM
408 FX(MF,JC)=(FM(MF)-FH(MF))/EY
YS(JC)=YS(JC)-EY
TM=TMM
PM=PMM
ZM=ZMM
IF (YS(JC)-0.9) 404,404,416
416 EY=-EY
404 CONTINUE
PRINT 12
PRINT 29
DO 409 MF=1,MX
FS=0.0
DO 410 JC=1,NC
410 FS=FS+YS(JC)*FX(MF,JC)
AUX=ALOG(ZN(MF)-BV(MF))
FYY(MF)=0.0
FWW(MF)=0.0
DO 411 JC=1,NC
FY(MF,JC)=FH(MF)+FX(MF,JC)-FS
FW(MF,JC)=(ZN(MF)-1.0)*BU(MF,JC)/BV(MF)-AUX-
2(AV(MF)/BV(MF))*(2.0*SQRT(AU(MF,JC)/AV(MF))-BU(MF,JC)/BV(MF))*
3ALOG(1.0+BV(MF)/ZN(MF))
411 CONTINUE
409 CONTINUE
DO 412 MF=1,MX
FDW=0.434294*FKH(MF)
FDY=0.434294*FH(MF)
FWD(1)=0.434294*FW(MF,1)
FYD(1)=0.434294*FY(MF,1)
FFW(1)=EXP(FW(MF,1))
FFY(1)=EXP(FY(MF,1))
PRINT 23,MF,TH(MF),PH(MF),FDW,FDY,FWD(1),FYD(1),FFW(1),FFY(1)
ND=NC-1
FWC(1)=YS(1)*FWD(1)
FYC(1)=YS(1)*FYD(1)
IF (NC-2) 413,413,414
414 DO 415 JC=2,ND
FWD(JC)=0.434294*FW(MF,JC)
FYD(JC)=0.434294*FY(MF,JC)
FWC(JC)=FWC(JC-1)+YS(JC)*FWD(JC)
```

```
FYC(JC)=FYC(JC-1)+YS(JC)*FYD(JC)
FFW(JC)=EXP(FW(MF,JC))
FFY(JC)=EXP(FY(MF,JC))
415 PRINT 24,FWD(JC),FYD(JC),FFW(JC),FFY(JC)
413 FWD(NC)=0.434294*FW(MF,NC)
FYD(NC)=0.434294*FY(MF,NC)
FWC(NC)=FWC(ND)+YS(NC)*FWD(NC)
FYC(NC)=FYC(ND)+YS(NC)*FYD(NC)
FFY(NC)=EXP(FY(MF,NC))
FFW(NC)=EXP(FW(MF,NC))
PRINT 25,FWC(NC),FYC(NC),FWD(NC),FYD(NC),FFW(NC),FFY(NC)
412 CONTINUE
KF=0
IF (KH-1) 97,501,97
C
C HEAT CONTENT, ENTROPY
501 KH=2
PRINT 12
PRINT 36
DO 503 MH=1,MX
503 TR(MH)=TR(MH)+ET
GO TO 504
502 DO 505 MH=1,MX
TR(MH)=TR(MH)-ET
HT=(FH(MH)-FM(MH))*TR(MH)/ET
SR=HT-FH(MH)-ALOG(PR(MH))
PLG=ALOG(PR(MH))
IF (KCL-9) 506,507,506
507 PRINT 37,MH,TH(MH),PH(MH),FH(MH),FM(MH),PLG,MTP(MH),MTPH(MH)
506 CONTINUE
505 PRINT 38,MH,TH(MH),PH(MH),TR(MH),PR(MH),HT,SR
KH=1
57 IF (KY) 98,98,108
98 READ 11,(TI(M),M=1,6),KCL,NC,NPC,NS,LAA,KE,EY,ET
IF (KCL) 99,101,101
99 STOP
END
```

Subroutine VIETA

SULFUR DIOXIDE				-0 1-012-0 5 -0.		-0.	
SD2	K AT	430.650000	77.808000			.269700	
H P.	TL	DT	DP				
-0 2 4	430.650000	92.500000	75.000000				

NC	T	P	TR	PR	ZK	ZF	LOG FK
1	430.650	75.000	1.000	.964	.476	.449	-.1680
2	430.650	150.000	1.000	1.928	.340	.278	-.3814
3	430.650	225.000	1.000	2.892	.459	.394	-.4878
4	430.650	300.000	1.000	3.856	.575	.508	-.5484
5	523.150	75.000	1.215	.964	.803	.809	-.0829
6	523.150	150.000	1.215	1.928	.614	.601	-.1693
7	523.150	225.000	1.215	2.892	.584	.568	-.2422
8	523.150	300.000	1.215	3.856	.643	.620	-.2910

NC	T	P	TR	PR	LOG FK	LOG FM	FK	FM
1	430.650	75.000	1.000	.964	-.1680	-.1749	.679	.668
2	430.650	150.000	1.000	1.928	-.3814	-.4109	.416	.388
3	430.650	225.000	1.000	2.892	-.4878	-.5286	.325	.296
4	430.650	300.000	1.000	3.856	-.5484	-.5975	.283	.253
5	523.150	75.000	1.215	.964	-.0829	-.0694	.826	.852
6	523.150	150.000	1.215	1.928	-.1693	-.1568	.677	.697
7	523.150	225.000	1.215	2.892	-.2422	-.2321	.573	.586
8	523.150	300.000	1.215	3.856	-.2910	-.2834	.512	.521

NC	T	P	TR	PR	HT	SR
1	430.650	75.000	1.000	.964	-1.9962	-1.5567
2	430.650	150.000	1.000	1.928	-4.6217	-4.3320
3	430.650	225.000	1.000	2.892	-4.8933	-4.7381
4	430.650	300.000	1.000	3.856	-4.8504	-4.8322
5	523.150	75.000	1.215	.964	-.7323	-.5358
6	523.150	150.000	1.215	1.928	-1.6987	-1.9940
7	523.150	225.000	1.215	2.892	-2.3484	-2.8757
8	523.150	300.000	1.215	3.856	-2.6394	-3.3363

ETHANE -0 1-012-0 5 -0. -0.
 C2H6 R PSIA 550.300000 715.500000 .285000

H P TL DT DP
 -0 3 5 559.680000 180.000000 2000.000000

NC	T	P	TR	PR	ZK	ZF	LOG FK
1	559.680	2000.000	1.017	2.795	.452	.404	-.4527
2	559.680	4000.000	1.017	5.590	.773	.745	-.5742
3	559.680	6000.000	1.017	8.386	1.072	1.072	-.5894
4	559.680	8000.000	1.017	11.181	1.360	1.386	-.5632
5	559.680	10000.000	1.017	13.976	1.638	1.688	-.5153
6	739.680	2000.000	1.344	2.795	.698	.693	-.1613
7	739.680	4000.000	1.344	5.590	.819	.807	-.2417
8	739.680	6000.000	1.344	8.386	1.024	1.012	-.2570
9	739.680	8000.000	1.344	11.181	1.235	1.226	-.2415
10	739.680	10000.000	1.344	13.976	1.444	1.439	-.2089
11	919.680	2000.000	1.671	2.795	.874	.885	-.0697
12	919.680	4000.000	1.671	5.590	.914	.928	-.1059
13	919.680	6000.000	1.671	8.386	1.043	1.052	-.1111
14	919.680	8000.000	1.671	11.181	1.196	1.202	-.0968
15	919.680	10000.000	1.671	13.976	1.355	1.359	-.0704

NC	T	P	TR	PR	LOG FK	LOG FM	FK	FM
1	559.680	2000.000	1.017	2.795	-.4527	-.4789	.353	.332
2	559.680	4000.000	1.017	5.590	-.5742	-.6124	.267	.244
3	559.680	6000.000	1.017	8.386	-.5894	-.6302	.257	.234
4	559.680	8000.000	1.017	11.181	-.5632	-.6024	.273	.250
5	559.680	10000.000	1.017	13.976	-.5153	-.5508	.305	.281
6	739.680	2000.000	1.344	2.795	-.1613	-.1546	.690	.701
7	739.680	4000.000	1.344	5.590	-.2417	-.2374	.573	.579
8	739.680	6000.000	1.344	8.386	-.2570	-.2549	.553	.556
9	739.680	8000.000	1.344	11.181	-.2415	-.2407	.574	.575
10	739.680	10000.000	1.344	13.976	-.2089	-.2088	.618	.618
11	919.680	2000.000	1.671	2.795	-.0697	-.0572	.852	.877
12	919.680	4000.000	1.671	5.590	-.1059	-.0897	.784	.813
13	919.680	6000.000	1.671	8.386	-.1111	-.0928	.774	.808
14	919.680	8000.000	1.671	11.181	-.0968	-.0775	.800	.837
15	919.680	10000.000	1.671	13.976	-.0704	-.0507	.850	.890

NC	T	P	TR	PR	HT	SR
1	559.680	2000.000	1.017	2.795	-4.1792	-4.1044
2	559.680	4000.000	1.017	5.590	-4.0692	-4.3801
3	559.680	6000.000	1.017	8.386	-3.9641	-4.6395
4	559.680	8000.000	1.017	11.181	-3.8482	-4.8754
5	559.680	10000.000	1.017	13.976	-3.6695	-5.0385
6	739.680	2000.000	1.344	2.795	-1.4789	-2.1509
7	739.680	4000.000	1.344	5.590	-2.0663	-3.2407
8	739.680	6000.000	1.344	8.386	-2.1751	-3.7147
9	739.680	8000.000	1.344	11.181	-2.1477	-4.0078
10	739.680	10000.000	1.344	13.976	-2.0559	-4.2126
11	919.680	2000.000	1.671	2.795	-1.6884	-1.5846
12	919.680	4000.000	1.671	5.590	-1.1236	-2.6382
13	919.680	6000.000	1.671	8.386	-1.3011	-3.2140

N-BUTANE-CARBON DIOXIDE -0 2-012-0 6 -0. -0.
 N-BUTANE R PSIA 765.310000 550.810000 .274000
 CARBON DIOXIDE R PSIA 547.490000 1070.160000 .274600
 -0. -0.

MOLE FRACTIONS
 2 .1000 .9000

TM PM ZM
 567.408745 946.933179 .274540

H P TL DT DP
 -0 3 5 559.680000 180.000000 2000.000000

NC	T	P	TR	PR	ZK	ZF	LOG FK
1	559.680	2000.000	.986	2.112	.358	.304	-.4293
2	559.680	4000.000	.986	4.224	.617	.564	-.5874
3	559.680	6000.000	.986	6.336	.860	.814	-.6347
4	559.680	8000.000	.986	8.448	1.091	1.055	-.6384
5	559.680	10000.000	.986	10.560	1.315	1.288	-.6190
6	739.680	2000.000	1.304	2.112	.696	.693	-.1415
7	739.680	4000.000	1.304	4.224	.713	.702	-.2385
8	739.680	6000.000	1.304	6.336	.865	.846	-.2771
9	739.680	8000.000	1.304	8.448	1.030	1.011	-.2842
10	739.680	10000.000	1.304	10.560	1.196	1.177	-.2735
11	919.680	2000.000	1.621	2.112	.875	.898	-.0624
12	919.680	4000.000	1.621	4.224	.859	.888	-.1052
13	919.680	6000.000	1.621	6.336	.933	.960	-.1248
14	919.680	8000.000	1.621	8.448	1.042	1.063	-.1268
15	919.680	10000.000	1.621	10.560	1.163	1.178	-.1171

NC	T	P	TR	PR	LOG FK	LOG FM	FK	FM
1	559.680	2000.000	.986	2.112	-.4293	-.4654	.372	.342
2	559.680	4000.000	.986	4.224	-.5874	-.6400	.259	.229
3	559.680	6000.000	.986	6.336	-.6347	-.6961	.232	.201
4	559.680	8000.000	.986	8.448	-.6384	-.7049	.230	.197
5	559.680	10000.000	.986	10.560	-.6190	-.6887	.240	.205
6	739.680	2000.000	1.304	2.112	-.1415	-.1286	.722	.744
7	739.680	4000.000	1.304	4.224	-.2385	-.2275	.577	.592
8	739.680	6000.000	1.304	6.336	-.2771	-.2688	.528	.539
9	739.680	8000.000	1.304	8.448	-.2842	-.2783	.520	.527
10	739.680	10000.000	1.304	10.560	-.2735	-.2695	.533	.538
11	919.680	2000.000	1.621	2.112	-.0624	-.0418	.866	.908
12	919.680	4000.000	1.621	4.224	-.1052	-.0767	.785	.838
13	919.680	6000.000	1.621	6.336	-.1248	-.0912	.750	.811
14	919.680	8000.000	1.621	8.448	-.1268	-.0902	.747	.812
15	919.680	10000.000	1.621	10.560	-.1171	-.0788	.764	.834

NC	T	P	LOG FW	LOG FYY	LOG FW	LOG FY	FW	FY
1	559.680	2000.000	-.4293	-.4654	-1.2476	-1.3649	.057	.043
			-.4293	-.4654	-.3383	-.3655	.459	.431
2	559.680	4000.000	-.5874	-.6400	-1.3142	-1.3934	.049	.040
			-.5874	-.6400	-.5067	-.5563	.311	.278
3	559.680	6000.000	-.6347	-.6961	-1.2535	-1.3467	.056	.045
			-.6347	-.6961	-.5660	-.6238	.272	.238
4	559.680	8000.000	-.6384	-.7049	-1.1458	-1.2353	.071	.058
			-.6384	-.7049	-.5820	-.6460	.262	.226
5	559.680	10000.000	-.6190	-.6887	-1.0142	-1.1015	.097	.079
			-.6190	-.6887	-.5751	-.6429	.266	.228
6	739.680	2000.000	-.1415	-.1286	-.4461	-.4546	.358	.351
			-.1415	-.1286	-.1076	-.0924	.780	.803
7	739.680	4000.000	-.2385	-.2275	-.6386	-.6671	.230	.215
			-.2385	-.2275	-.1941	-.1787	.640	.663
8	739.680	6000.000	-.2771	-.2688	-.6364	-.6794	.231	.209
			-.2771	-.2688	-.2372	-.2232	.579	.598
9	739.680	8000.000	-.2842	-.2783	-.5759	-.6244	.266	.237
			-.2842	-.2783	-.2518	-.2398	.560	.576
10	739.680	10000.000	-.2735	-.2695	-.4890	-.5410	.324	.288
			-.2735	-.2695	-.2496	-.2393	.563	.576
11	919.680	2000.000	-.0624	-.0418	-.1963	-.1740	.636	.670
			-.0624	-.0418	-.0475	-.0271	.896	.940
12	919.680	4000.000	-.1052	-.0767	-.3056	-.2850	.495	.519
			-.1052	-.0767	-.0830	-.0536	.826	.884
13	919.680	6000.000	-.1248	-.0912	-.3216	-.3094	.477	.490
			-.1248	-.0912	-.1029	-.0669	.789	.857
14	919.680	8000.000	-.1268	-.0902	-.2870	-.2859	.516	.518
			-.1268	-.0902	-.1090	-.0685	.778	.854
15	919.680	10000.000	-.1171	-.0788	-.2265	-.2350	.594	.582
			-.1171	-.0788	-.1050	-.0615	.785	.868

NC	T	P	TR	PR	HT	SR
1	559.680	2000.000	.986	2.112	-4.3476	-4.0236
2	559.680	4000.000	.986	4.224	-4.3073	-4.2745
3	559.680	6000.000	.986	6.336	-4.3426	-4.5861
4	559.680	8000.000	.986	8.448	-4.2222	-4.7329
5	559.680	10000.000	.986	10.560	-4.0976	-4.8689
6	739.680	2000.000	1.304	2.112	-1.3451	-1.7966
7	739.680	4000.000	1.304	4.224	-2.1702	-3.0871
8	739.680	6000.000	1.304	6.336	-2.4031	-3.6305
9	739.680	8000.000	1.304	8.448	-2.4556	-3.9487
10	739.680	10000.000	1.304	10.560	-2.4354	-4.1720
11	919.680	2000.000	1.621	2.112	-.6054	-1.2569
12	919.680	4000.000	1.621	4.224	-1.1116	-2.3757
13	919.680	6000.000	1.621	6.336	-1.4005	-3.0369
14	919.680	8000.000	1.621	8.448	-1.5524	-3.4786
15	919.680	10000.000	1.621	10.560	-1.6232	-3.7988

MOLE FRACTIONS
1 .5000 .5000

TM PM ZM
654.911539 689.357782 .274300

H P TL DT DP
-0 3 5 559.680000 180.000000 2000.000000

NC	T	P	TR	PR	ZK	ZF	LOG FK
1	559.680	2000.000	.855	2.901	.447	.413	-.7966
2	559.680	4000.000	.855	5.803	.832	.789	-.9109
3	559.680	6000.000	.855	8.704	1.193	1.143	-.9106
4	559.680	8000.000	.855	11.605	1.541	1.481	-.8656
5	559.680	10000.000	.855	14.506	1.879	1.804	-.7974
6	739.680	2000.000	1.129	2.901	.518	.489	-.3184
7	739.680	4000.000	1.129	5.803	.796	.765	-.4271
8	739.680	6000.000	1.129	8.704	1.073	1.048	-.4401
9	739.680	8000.000	1.129	11.605	1.341	1.322	-.4149
10	739.680	10000.000	1.129	14.506	1.601	1.589	-.3697
11	919.680	2000.000	1.404	2.901	.741	.747	-.1411
12	919.680	4000.000	1.404	5.803	.850	.845	-.2099
13	919.680	6000.000	1.404	8.704	1.048	1.036	-.2204
14	919.680	8000.000	1.404	11.605	1.255	1.241	-.2022
15	919.680	10000.000	1.404	14.506	1.460	1.447	-.1679

NC	T	P	TR	PR	LOG FK	LOG FM	FK	FM
1	559.680	2000.000	.855	2.901	-.7966	-.9234	.160	.119
2	559.680	4000.000	.855	5.803	-.9109	-1.0494	.123	.089
3	559.680	6000.000	.855	8.704	-.9106	-1.0572	.123	.088
4	559.680	8000.000	.855	11.605	-.8656	-1.0190	.136	.096
5	559.680	10000.000	.855	14.506	-.7974	-.9572	.159	.110
6	739.680	2000.000	1.129	2.901	-.3184	-.3207	.480	.478
7	739.680	4000.000	1.129	5.803	-.4271	-.4387	.374	.364
8	739.680	6000.000	1.129	8.704	-.4401	-.4567	.363	.349
9	739.680	8000.000	1.129	11.605	-.4149	-.4343	.385	.368
10	739.680	10000.000	1.129	14.506	-.3697	-.3905	.427	.407
11	919.680	2000.000	1.404	2.901	-.1411	-.1244	.723	.751
12	919.680	4000.000	1.404	5.803	-.2099	-.1926	.617	.642
13	919.680	6000.000	1.404	8.704	-.2204	-.2047	.602	.624
14	919.680	8000.000	1.404	11.605	-.2022	-.1880	.628	.649
15	919.680	10000.000	1.404	14.506	-.1679	-.1550	.679	.700

NC	T	P	LOG FW	LOG FYY	LOG FW	LOG FY	FW	FY
1	559.680	2000.000	-.7966	-.9234	-1.2583	-1.3745	.055	.042
			.7966	-.9234	-.3350	-.4724	.462	.337
2	559.680	4000.000	-.9109	-1.0494	-1.3157	-1.4473	.048	.036
			-.9109	-1.0494	-.5061	-.6515	.312	.223
3	559.680	6000.000	-.9106	-1.0572	-1.2561	-1.4038	.055	.039
			-.9106	-1.0572	-.5651	-.7106	.272	.195
4	559.680	8000.000	-.8656	-1.0190	-1.1511	-1.3159	.071	.048

			-.8656	-1.0190	-.5802	-.7222	.263	.190
5	559.680	10000.000	-.7974	-.9572	-1.0225	-1.2062	.095	.062
			-.7974	-.9572	-.5723	-.7083	.268	.196
6	739.680	2000.000	-.3184	-.3207	-.5784	-.6086	.264	.246
			-.3184	-.3207	-.0583	-.0327	.874	.927
7	739.680	4000.000	-.4271	-.4387	-.6709	-.7135	.213	.193
			-.4271	-.4387	-.1832	-.1639	.656	.686
8	739.680	6000.000	-.4401	-.4567	-.6464	-.6951	.226	.202
			-.4401	-.4567	-.2337	-.2183	.584	.605
9	739.680	8000.000	-.4149	-.4343	-.5792	-.6300	.264	.234
			-.4149	-.4343	-.2506	-.2386	.562	.577
10	739.680	10000.000	-.3697	-.3905	-.4903	-.5413	.323	.288
			-.3697	-.3905	-.2491	-.2397	.564	.576
11	919.680	2000.000	-.1411	-.1244	-.2642	-.2575	.544	.553
			-.1411	-.1244	-.0179	.0088	.960	1.020
12	919.680	4000.000	-.2099	-.1926	-.3560	-.3594	.441	.437
			-.2099	-.1926	-.0639	-.0259	.863	.942
13	919.680	6000.000	-.2204	-.2047	-.3472	-.3576	.450	.439
			-.2204	-.2047	-.0937	-.0517	.806	.888
14	919.680	8000.000	-.2022	-.1880	-.2999	-.3149	.501	.484
			-.2022	-.1880	-.1044	-.0612	.786	.869
15	919.680	10000.000	-.1679	-.1550	-.2331	-.2507	.585	.561
			-.1679	-.1550	-.1026	-.0594	.790	.872

NG	T	P	TR	PR	HT	SR
1	559.680	2000.000	.855	2.901	-5.6091	-4.5479
2	559.680	4000.000	.855	5.803	-5.5314	-4.8734
3	559.680	6000.000	.855	8.704	-5.4416	-5.1711
4	559.680	8000.000	.855	11.605	-5.2847	-5.3897
5	559.680	10000.000	.855	14.506	-5.1889	-5.6594
6	739.680	2000.000	1.129	2.901	-3.0106	-3.3374
7	739.680	4000.000	1.129	5.803	-3.2950	-4.0432
8	739.680	6000.000	1.129	8.704	-3.2857	-4.3979
9	739.680	8000.000	1.129	11.605	-3.1778	-4.6293
10	739.680	10000.000	1.129	14.506	-3.0261	-4.8014
11	919.680	2000.000	1.404	2.901	-1.3602	-2.1390
12	919.680	4000.000	1.404	5.803	-1.9824	-3.2971
13	919.680	6000.000	1.404	8.704	-2.1324	-3.8249
14	919.680	8000.000	1.404	11.605	-2.1290	-4.1475
15	919.680	10000.000	1.404	14.506	-2.0601	-4.3777

MOLE FRACTIONS
-0.9000 .1000

			TM	PM	ZM		
			743.528451	571.298732	.274060		
	H P	TL	DT	DP			
	-0 3 5	559.680000	180.000000	2000.000000			
NC	T	P	TR	PR	ZK	ZF	LOG FK
1	559.680	2000.000	.753	3.501	.550	.487	-1.1667

2	559.680	4000.000	.753	7.002	1.048	.933	-1.2350
3	559.680	6000.000	.753	10.502	1.523	1.352	-1.1872
4	559.680	8000.000	.753	14.003	1.982	1.752	-1.0945
5	559.680	10000.000	.753	17.504	2.432	2.137	-.9783
6	739.680	2000.000	.995	3.501	.532	.474	-.5382
7	739.680	4000.000	.995	7.002	.931	.885	-.6249
8	739.680	6000.000	.995	10.502	1.304	1.274	-.6061
9	739.680	8000.000	.995	14.003	1.662	1.644	-.5467
10	739.680	10000.000	.995	17.504	2.009	1.999	-.4663
11	919.680	2000.000	1.237	3.501	.632	.615	-.2582
12	919.680	4000.000	1.237	7.002	.911	.887	-.3335
13	919.680	6000.000	1.237	10.502	1.206	1.185	-.3248
14	919.680	8000.000	1.237	14.003	1.494	1.478	-.2818
15	919.680	10000.000	1.237	17.504	1.775	1.764	-.2208

NO	T	P	TR	PR	LOG FK	LOG FM	FK	FM
1	559.680	2000.000	.753	3.501	-1.1667	-.9619	.068	.109
2	559.680	4000.000	.753	7.002	-1.2350	-1.0562	.058	.088
3	559.680	6000.000	.753	10.502	-1.1872	-1.0332	.065	.093
4	559.680	8000.000	.753	14.003	-1.0945	-.9652	.080	.108
5	559.680	10000.000	.753	17.504	-.9783	-.8743	.105	.134
6	739.680	2000.000	.995	3.501	-.5382	-.5878	.290	.258
7	739.680	4000.000	.995	7.002	-.6249	-.6905	.237	.204
8	739.680	6000.000	.995	10.502	-.6061	-.6785	.248	.210
9	739.680	8000.000	.995	14.003	-.5467	-.6221	.284	.239
10	739.680	10000.000	.995	17.504	-.4663	-.5431	.342	.286
11	919.680	2000.000	1.237	3.501	-.2582	-.2523	.552	.559
12	919.680	4000.000	1.237	7.002	-.3335	-.3341	.464	.463
13	919.680	6000.000	1.237	10.502	-.3248	-.3294	.473	.468
14	919.680	8000.000	1.237	14.003	-.2818	-.2888	.523	.514
15	919.680	10000.000	1.237	17.504	-.2208	-.2291	.601	.590

NO	T	P	LOG FW	LOG FYY	LOG FW	LOG FY	FW	FY
1	559.680	2000.000	-1.1667	-.9619	-1.2594	-1.0880	.055	.082
			-1.1667	-.9619	-.3328	.1728	.465	1.489
2	559.680	4000.000	-1.2350	-1.0562	-1.3160	-1.1788	.048	.066
			-1.2350	-1.0562	-.5056	.0475	.312	1.116
3	559.680	6000.000	-1.1872	-1.0332	-1.2564	-1.1522	.055	.070
			-1.1872	-1.0332	-.5643	.0370	.273	1.089
4	559.680	8000.000	-1.0945	-.9652	-1.1518	-1.0802	.071	.083
			-1.0945	-.9652	-.5788	.0693	.264	1.173
5	559.680	10000.000	-.9783	-.8743	-1.0236	-.9850	.095	.104
			-.9783	-.8743	-.5701	.1222	.269	1.325
6	739.680	2000.000	-.5382	-.5878	-.5950	-.6504	.254	.224
			-.5382	-.5878	-.0267	-.0244	.940	.945
7	739.680	4000.000	-.6249	-.6905	-.6748	-.7441	.211	.180
			-.6249	-.6905	-.1754	-.2084	.668	.619
8	739.680	6000.000	-.6061	-.6785	-.6478	-.7230	.225	.189
			-.6061	-.6785	-.2309	-.2776	.588	.528
9	739.680	8000.000	-.5467	-.6221	-.5797	-.6579	.263	.220
			-.5467	-.6221	-.2495	-.3000	.563	.501
10	739.680	10000.000	-.4663	-.5431	-.4905	-.5704	.323	.269

			-.4663	-.5431	-.2486	-.2970	.564	.505
11	919.680	2000.000	-.2582	-.2523	-.2915	-.2889	.511	.514
			-.2582	-.2523	.0417	.0773	1.101	1.195
12	919.680	4000.000	-.3335	-.3341	-.3657	-.3708	.431	.426
			-.3335	-.3341	-.0441	-.0038	.903	.991
13	919.680	6000.000	-.3248	-.3294	-.3514	-.3605	.445	.436
			-.3248	-.3294	-.0850	-.0502	.822	.891
14	919.680	8000.000	-.2818	-.2888	-.3020	-.3133	.499	.486
			-.2818	-.2888	-.1001	-.0684	.794	.854
15	919.680	10000.000	-.2208	-.2291	-.2342	-.2466	.583	.567
			-.2208	-.2291	-.1004	-.0715	.794	.848

NC	T	P	TR	PR	HT	SR
1	559.680	2000.000	.753	3.501	-9.2259	-8.2640
2	559.680	4000.000	.753	7.002	-9.5309	-9.0451
3	559.680	6000.000	.753	10.502	-9.7802	-9.7527
4	559.680	8000.000	.753	14.003	-9.9842	-10.4009
5	559.680	10000.000	.753	17.504	-10.1486	-10.9979
6	739.680	2000.000	.995	3.501	-4.4310	-4.3306
7	739.680	4000.000	.995	7.002	-4.1817	-4.5378
8	739.680	6000.000	.995	10.502	-3.9756	-4.7649
9	739.680	8000.000	.995	14.003	-3.7673	-4.9741
10	739.680	10000.000	.995	17.504	-3.5625	-5.1745
11	919.680	2000.000	1.237	3.501	-2.3663	-3.0384
12	919.680	4000.000	1.237	7.002	-2.7244	-3.9012
13	919.680	6000.000	1.237	10.502	-2.6917	-4.2848
14	919.680	8000.000	1.237	14.003	-2.5582	-4.5325
15	919.680	10000.000	1.237	17.504	-2.3815	-4.7163

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