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LOS ALAMOS SCIENTIFIC LABORATORY
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LOS ALAMOS • NEW MEXICO

FORTRAN BKW:
A Code for Computing the Detonation Properties of Explosives

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by

Charles L. Mader

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FORTRAN BKW
A CODE FOR COMPUTING THE DETONATION PROPERTIES OF EXPLOSIVES

by

Charles L. Mader

ABSTRACT

This report describes a FORTRAN code for the CDC 6600 computer. The code computes the steady-state detonation properties of an explosive using the Becker-Kistiakowsky-Wilson equation of state.

I. INTRODUCTION. The Becker-Kistiakowsky-Wilson equation of state has been described and calibrated by the author.[1-3] An internal report,[2] written in 1962, described the STRETCH BKW code which was written in machine language for the IBM 7030. The present report describes a similar code recently written in FORTRAN IV language for the CDC 6600. The code was written, as far as possible, to use input identical to and give output similar to the STRETCH BKW code. Though one can not determine the nature of a future FORTRAN language, an attempt has been made to use the more general FORTRAN expressions and formats rather than the features special to CDC 6600 FORTRAN. The code is sufficiently general that it will also run on the IBM 7030.

FORTRAN BKW is a code for computing the detonation properties of an explosive using the Becker-Kistiakowsky-Wilson equation of state.[1-3] One may also compute the Hugoniot; the isentrope through the computed C-J value; the coefficients to fits of the pressure, volume, energy, and temperature along the isentrope; and the particle velocity along the isentrope. Fits of the results are computed for use in the HOM[4] equation of state subroutine used in reactive hydrodynamic codes. The output is available both as printed listings and on microfilm. Graphs of Hugoniot pressure vs. volume, pressure vs. particle velocity, shock vs. particle velocity, isentrope pressure vs. volume, temperature vs. volume, and particle velocity vs. pressure are also available on microfilm.

FORTRAN BKW includes an equilibrium subroutine that can solve the equilibrium composition of a system of 10 elements, 20 gaseous species, and five other phases subject to the limitation that only one phase may disappear.

For the explosive the calculation requires as input data its elemental composition, heat of formation, density, and formula weight; and for the gaseous explosion products, their elemental compositions, heats of formation, covolumes, and quartic fits of their ideal gas entropies as a function of temperature. For the solid explosion products, the calculation also requires the density, molecular weight, and (if the solid is to be considered compressible) the parameters in the Cowan solid equation of state.[5] The only initial guesses required are the number of moles of each of the explosion products. The iteration procedures should give all values to 1 in 10^5. Some differences will be noticed between STRETCH BKW and FORTRAN BKW output in the sixth significant figure because of round-off error.

We shall present the input and output for a typical problem and then a detailed description of the coding formulas. A knowledge of FORTRAN IV is assumed.

II. NOMENCLATURE.

α	BKW equation of state constant = 0.5
β	BKW equation of state constant = 0.16
θ	BKW equation of state constant = 400
K	BKW equation of state constant = 10.9097784436
M	Number of elements in the explosive
N	Number of gaseous species in detonation products
NT	Total number of species in detonation products
T	Temperature in °K
P	Pressure in Mbar
SO or S^o	Entropy in cal/deg-mole
A B C D E	Coefficients to entropy fit SO = A + $BT + CT^2 + DT^3 + ET^4$
(H - HO)	Enthalpy in cal/mole
(F - HO)/T	Free energy in cal/deg-mole
IC	Integration constant for forming (H - HO) and (F - HO)/T from SO fit
A_s, A1 B_s, A2 C_s, C1 D_s, C2 E_s, C3	Coefficients to Cowan solid equation of state
$(\Delta H_f^o)_i$	Heat of formation at 0°K of component i in cal/mole
V_o	$1/\rho_o$ where ρ_o = density in g/cc
V_o'	$1/\rho_o$ where ρ_o = density of explosive in g/cc
X_i	Number of moles of ith species per mole of explosive
Y_i	X_i one step earlier in the same subroutine
α_{ik}	Input detonation product elemental composition matrix
b_k	Input explosive elemental composition vector
ρ_s	Density of solid in g/cc
T_v	Temperature in volts
D	Detonation velocity in cm/μsec
V_g	Volume of the gas in cc/mole
V_s	Volume of solid in cc/g
k_i	Covolume
R_1	1.98718
R_2	8.341439×10^{-5}
R_3	2.39004905×10^4
R_4	0.98692×10^6
R_5	11,605.6
R_6	0.4342944819
f_i	Total free energy of gas
$(G)_i$	Total free energy of solid
F'_s	Imperfection solid free energy
E'_s	Imperfection solid enthalpy
S'_s	Imperfection solid entropy
E'_g	Imperfection gas enthalpy
S'_g	Imperfection gas entropy
E_g	Total enthalpy of gas
$(E_s)_i$	Total enthalpy of solid i
MOLWT	Molecular weight of a solid
AMOLWT	Explosive formula weight
E_{Total}	Energy in cal/mole
V_{Total}	Volume in cc/mole of explosive
VPG	Volume in cc/g of explosive
E_o	Heat of formation of explosive
IND	Error indicator
U_s	Shock velocity
U_p	Particle velocity

III. FORTRAN BKW INPUT.

The input of a FORTRAN BKW calculation of RDX at a density of 1.8 g/cc is described in detail. The input is identical to that used for RDX in Reference 3. Below is a description of the loading form which immediately follows.

Card 1 (Format I5) 0 = NO, 1 = YES

Column	
2-5	Perform a single equilibrium calculation for input T, P
7-10	Perform the C-J calculation
12-15	Perform the Hugoniot calculation (1 must be in column 10)
17-20	Perform the isentrope calculation through the computed C-J point (1 must be in column 10)
22-25	Give microfilm output
27-30	Ignored
32-35	Perform the calculation for this number of other densities (Max of 4)
37-40	Ignored
42-45	Ignored
47-50	Number of extra data cards

Card 2 (Format 12A6)

Column	
2-72	Name of explosive

Card 3 (Format 3I5)

Column	
2-5	Number of elements in explosive = (M)
7-10	Number of gaseous species = (N)
12-15	Total number of gaseous and solid species = (NT)

Card 4 (Format 4E18.11)

Column	
1-18	BKW equation of state α
19-36	BKW equation of state β
37-54	BKW equation of state θ
55-72	BKW equation of state K

All floating-point input will follow the form of Card 4.

Card 5 (Format 11A6)
The empirical formula of the explosive

Column	
2-6	Symbol of 1st element
8-12	Symbol of 2nd element
14-18	Symbol of 3rd element
20-24	Symbol of Mth element since M = 4 (Max of 10)

Card 6 (Format 4E18.11)

Column	
1-18	G-atoms of 1st element/formula weight
19-36	G-atoms of 2nd element/formula weight
37-54	G-atoms of 3rd element/formula weight
55-72	G-atoms of Mth element/formula weight since M = 4 (Max of 10)

Card 7 (Format 4E18.11)

Column	
1-18	Density of explosive (g/cc)
19-36	Formula weight (grams)
37-54	Heat of formation at 0°K (cal/formula weight)

Card 8 (Format 4E18.11)

Column	
1-18	Temperature (°K)
19-36	Pressure (Mbar)

This card must be present; however, if column 2-5 of Card 1 is zero, it is not used by the code.

Card 9 (Format 11A6)

Column	
2-6	Symbol of 1st gas species
8-12	Symbol of 2nd gas species
14-18, 20-24, 26-30, 32-36, 38-42, 44-48, 50-54, 56-60, 62-66	Symbol of Nth gas species

Card 10 (Format 11A6)

Column	
2-6	Symbol of 1st solid species (This is on new card because previous card is full at 11)

Rules
1. All gas species first (Max of 20)
2. Then solid species (Max of 5)
3. Only 11 sets of symbols per card

Cards 11, 12, 13 - (NT floating-point numbers)

Moles of each species (in same order as in Card 9) per formula weight (Guesses).

Cards 14 through 37 - A total of (NT)*(8) floating-point numbers

Nos.1-5 The coefficients A, B, C, D, E to the fit SO (cal/mole-°K) = $A + BT + CT^2 + DT^3 + ET^4$

No.6 Then the integration constant from

$$H - HO(\text{cal/mole}) = \frac{BT^2}{2} + \frac{2CT^3}{3} + \frac{3DT^4}{4} + \frac{4ET^5}{5} + IC$$

at some temperature (we used 2500°K in example)

No.7 Then the heat of formation in cal/mole

No.8 Then the covolume (see Reference 3 for details)

Thus eight numbers on two cards for each species and each species in same order as Cards 9,10.

Card 38 (Format 11A6)

Column	
2-6	Symbol of 1st solid phase (Max of 5)

Cards 39-40-41 (NT-N)*(12) numbers

No. 1 VO (cc/g)

Nos. 2-11 If VO (No. 1) is zero, the solid will be treated as incompressible and all the rest of the numbers will be ignored except the last one (molecular weight); however, cards must be present for all 10 numbers. Otherwise the coefficients to the Cowan-Fickett solid equation of state are punched as follows:

A_s, B_s, C_s, D_s, E_s, A1, A2, C1, C2, C3

No. 12 Molecular weight

(Max of five sets in same order as Card 38)

Cards 42-53 (M)*(NT) numbers

The input detonation product elemental composition matrix

$$\begin{array}{c|cccc} & C & H & N & O \\ \hline H_2O & 0 & 2 & 0 & 1 \\ H_2 & 0 & 2 & 0 & 0 \\ O_2 & 0 & 0 & 0 & 2 \\ & \text{etc.} & & & \end{array}$$

given by row sequentially as

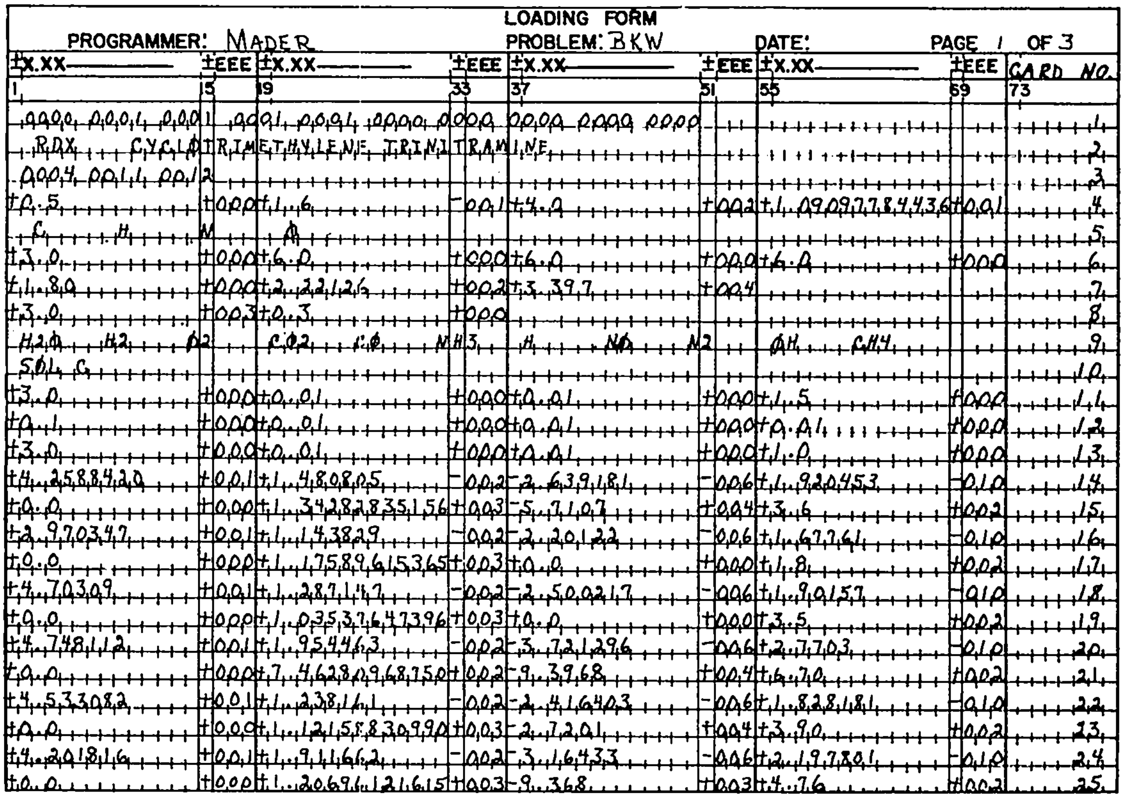
0, 2, 0, 1, 0, 2, 0, 0, 0, 0, 0, 2, etc.

Other Optional Input

Card A. If column 35 of Card 1 is > 0 ≤ 4, that number of densities are read and the requested calculations are performed for each density. One card with a maximum of four floating-point numbers if column 35 > 0.

Card B. If column 49-50 of card 1 is > 0 < 25, the code expects that number of cards of the format (1I5, 1E18.11) where I5 is the format of the constant identity number and the 1E18.11 is the format of the new constant as described in Section VI. If column 49-50 of card 1 is 0 no cards of this type are present.

After completion of the calculation for one explosive, the calculation reads in the next set of input starting with 1.



LOADING FORM

PROGRAMMER: MADER PROBLEM: BKW DATE: PAGE 1 OF 3

±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	CARD NO.
1	15	19	33	37	51	55	69	73
0000 0001 000	1 00	01 0001 0000 0	000	0000 0000 0000				1
RDX CYCLO	TRIM	ETHYLENE TRINI	TRAM	INE				2
0004 0011 001	2							3
+0.5	+000	+1.6	-001	+4.0	+002	+1.09097784436	+001	4
C H	N	O						5
+3.0	+000	+6.0	+000	+6.0	+000	+6.0	+000	6
+1.80	+000	+2.22126	+002	+3.397	+004			7
+3.0	+003	+0.3	+000					8
H2O H2 O	2	CO2 CO N	H3	H NO N	2	OH CH4		9
SOL C								10
+3.0	+000	+0.01	+000	+0.01	+000	+1.5	+000	11
+0.1	+000	+0.01	+000	+0.01	+000	+0.01	+000	12
+3.0	+000	+0.01	+000	+0.01	+000	+1.0	+000	13
+4.2588420	+001	+1.48085	-002	-2.639181	-006	+1.920453	-010	14
+0.0	+000	+1.34282835156	+003	-5.7107	+004	+3.6	+002	15
+2.970347	+001	+1.143829	-002	-2.20122	-006	+1.67761	-010	16
+0.0	+000	+1.17589615365	+003	+0.0	+000	+1.8	+002	17
+4.70309	+001	+1.287147	-002	-2.500217	-006	+1.90157	-010	18
+0.0	+000	+1.03537647396	+003	+0.0	+000	+3.5	+002	19
+4.748112	+001	+1.954463	-002	-3.721296	-006	+2.7703	-010	20
+0.0	+000	+7.46280968750	+002	-9.3968	+004	+6.70	+002	21
+4.533082	+001	+1.238161	-002	-2.416403	-006	+1.828181	-010	22
+0.0	+000	+1.12155830990	+003	-2.7201	+004	+3.90	+002	23
+4.201816	+001	+1.911662	-002	-3.16433	-006	+2.197801	-010	24
+0.0	+000	+1.20696121615	+003	-9.368	+003	+4.76	+002	25

LOADING FORM

PROGRAMMER: MADER PROBLEM: DATE: PAGE 2 OF 3

±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	CARD NO.
1	15	19	33	37	51	55	69	73
+2.63911	+001	+8.121372	-003	-1.69074	-006	+1.318623	-010	26
+0.0	+000	+7.9463161718 8	+002	+5.1619	+004	+7.6	+001	27
+4.841498	+001	+1.269386	-002	-2.4946	-006	+1.893213	-010	28
+0.0	+000	+1.2092497057 3	+003	+2.14770	+004	+3.86	+002	29
+4.39234	+001	+1.222501	-002	-2.379005	-006	+1.798322	-010	30
+0.0	+000	+1.1391613489 6	+003	+0.0	+000	+3.8	+002	31
+4.241792	+001	+1.156847	-002	-2.226659	-006	+1.689155	-010	32
+0.0	+000	+1.1835175442 7	+003	+3.56	+003	+4.13	+002	33
+3.875686	+001	+2.364013	-002	-3.707957	-006	+2.470714	-010	34
+0.0	+000	+1.0424279114 6	+003	-1.6	+004	+5.28	+002	35
-2.461519	-001	+7.179855	-003	-1.29755	-006	+9.349995	-011	36
+0.0	+000	-2.5820438932 3	+002	+0.0	+000	+0.0	+000	37
SØL C								38
+4.4444444444 4	-001	+8.3093583726 8	-001	-1.3938180921 9	+000	+6.7256971602 1	-001	39
-1.1353726250 8	-001	+6.4915588200 7	-003	-2.2670534594 8	-001	+1.2051656952 5	-001	40
+8.316	-002	-1.7559	-001	+1.5531	-001	+1.201	+001	41
+0.0	+000	+2.0	+000	+0.0	+000	+1.0	+000	42
+0.0	+000	+2.0	+000	+0.0	+000	+0.0	+000	43
+0.0	+000	+0.0	+000	+0.0	+000	+2.0	+000	44
+1.0	+000	+0.0	+000	+0.0	+000	+2.0	+000	45
+1.0	+000	+0.0	+000	+0.0	+000	+1.0	+000	46
+0.0	+000	+3.0	+000	+1.0	+000	+0.0	+000	47
+0.0	+000	+1.0	+000	+0.0	+000	+0.0	+000	48
+0.0	+000	+0.0	+000	+1.0	+000	+1.0	+000	49
+0.0	+000	+0.0	+000	+2.0	+000	+0.0	+000	50

LOADING FORM

PROGRAMMER: MADER PROBLEM: DATE: PAGE 3 OF 3

±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	±X.XX	±EEE	CARD NO.
1	15	19	33	37	51	55	69	73
+0.0	+000	+1.0	+000	+0.0	+000	+1.0	+000	51
+1.0	+000	+4.0	+000	+0.0	+000	+0.0	+000	52
+1.0	+000	+0.0	+000	+0.0	+000	+0.0	+000	53
+1.6	+000	+1.4	+000	+1.2	+000	+1.0	+000	A
0012+2.5		-001						B

IV. <u>FORTRAN BKW OUTPUT.</u> This section presents the output of FORTRAN BKW for the input just given. The equations found by fitting the isentrope data are of the form

$$\ln(P) = A' = B'(\ln V) + C'(\ln V)^2 + D'(\ln V)^3 + E'(\ln V)^4$$

where $(\ln V)^4$ is written as LNV*4. The units on the graphs are the same as those in the listings.

The CDC 6600 machine time required for the example was:

The C-J value	22.8 seconds
The nine Hugoniot points	27.5 seconds
The isentrope calculation	78.9 seconds

Smaller product sets take less time. If a solid phase disappears, the time is considerably longer.

```
 A FORTRAN BKW CALCULATION FOR THE EXPLOSIVE
 RDX       CYCLOTRIMETHYLENE TRINITRAMINE


THE NUMBER OF ELEMENTS IS       4


THE NUMBER OF GAS SPECIES IS    11


THE NUMBER OF SOLID SPECIES IS     1


THE BKW EQUATION OF STATE PARAMETERS ARE
 ALPHA= 5.00000000000E-01 BETA= 1.60000000000E-01 THETA= 4.00000000000E+02 KAPPA= 1.09097784436E+01


THE COMPOSITION OF THE EXPLOSIVE IS
     3.00000000000E+00 MOLES OF   C
     6.00000000000E+00 MOLES OF   H
     6.00000000000E+00 MOLES OF   N
     6.00000000000E+00 MOLES OF   O


THE DENSITY OF THE EXPLOSIVE IS  1.80000000000E+00, GRAMS/CC


THE MOLECULAR WEIGHT IS  2.22126000000E+02 GRAMS


THE HEAT OF FORMATION AT 0 DEG K IS  3.39700000000E+04 CALORIES PER FORMULA WEIGHT


THE SOLID (COWAN) EQUATION OF STATE PARAMETERS    VO, AS, BS, CS, DS, ES,     A1, A2, C1, C2, C3, ATOMIC WT


SOL C   4.44444444444E-01   8.50935837268E-01  -1.39381809219E+00   6.72569716021E-01  -1.13537262508E-01   6.49155882007E-03
       -2.26705345948E-01   1.20516569525E-01   8.31600000000E-02  -1.75590000000E-01   1.55310000000E-01   1.20100000000E+01


THE INPUT DETONATION PRODUCT ELEMENTAL COMPOSITION MATRIX
  0          2.0E+00    0          1.0E+00    0          2.0E+00    0          0          0          0          0          2.0E+00
  1.0E+00    0          0          2.0E+00    1.0E+00    0          0          1.0E+00    0          3.0E+00    1.0E+00    0
  0          1.0E+00    0          0          0          0          1.0E+00    1.0E+00    0          0          2.0E+00    0
  0          1.0E+00    0          1.0E+00    1.0E+00    4.0E+00    0          0          1.0E+00    0          0          0
```

```
A FORTRAN BKW CALCULATION FOR THE EXPLOSIVE
RDX        CYCLOTRIMETHYLENE TRINITRAMINE


THE COMPUTED CJ PRESSURE IS     3.46662648781E-01     MEGABARS


THE COMPUTED DETONATION VELOCITY IS     8.75399404525E-01     CM/MICROSECOND


THE COMPUTED CJ TEMPERATURE IS     2.58759366556E+03     DEGREES KELVIN


THE COMPUTED CJ VOLUME     4.15935343157E-01  CC/GM OF EXPLOSIVE


THE COMPUTED GAMMA IS  2.97903672705E+00


THE VOLUME OF THE GAS IS     1.16225961323E+01    CC/MOLE OF GAS AND THERE ARE     7.51092369275E+00    MOLES OF GAS


SOLID      VOLUME IN CC/GM
SOL C      2.84815647821E-01


THE C-J COMPOSITION OF THE DETONATION PRODUCTS AND THE INPUT COEFFICIENTS TO THE THERMODYNAMIC FITS FOR EACH SPECIE


SPECIE     NO OF MOLES          COEFFICIENTS A,B,C,D,E, THE INTEGRATION CONSTANT, HEAT OF FORMATION IN CAL/MOLE,COVOLUME
H2O        2.99994556597E+00    4.25884200000E+01    1.48080500000E-02   -2.63918100000E-06    1.92045300000E-10    0.
                                1.34282835156E+03   -5.71070000000E+04    2.50000000000E+02
H2         9.45374846362E-06    2.97034700000E+01    1.14382900000E-02   -2.20122200000E-06    1.67776100000E-10    0.
                                1.17589615365E+03    0.                   1.80000000000E+02
O2         2.88697862711E-06    4.70309000000E+01    1.28714700000E-02   -2.50021700000E-06    1.90157000000E-10    0.
                                1.03537647396E+03    0.                   3.50000000000E+02
CO2        1.48906096263E+00    4.74811200000E+01    1.95446300000E-02   -3.72129600000E-06    2.77030000000E-10    0.
                                7.46280968750E+02   -9.39680000000E+04    6.00000000000E+02
CO         2.18525884702E-02    4.53308200000E+01    1.23816100000E-02   -2.41640300000E-06    1.82818100000E-10    0.
                                1.12158830990E+03   -2.72010000000E+04    3.90000000000E+02
NH3        7.95040784085E-05    4.20181600000E+01    1.91166200000E-02   -3.16433000000E-06    2.19780100000E-10    0.
                                1.20696121615E+03   -9.36800000000E+03    4.76000000000E+02
H          5..9647876225E-10    2.63911000000E+01    8.12137200000E-03   -1.69074000000E-06    1.31682300000E-10    0.
                                7.94631617188E+02    5.16190000000E+04    7.60000000000E+01
NO         7.41458015996E-05    4.84149800000E+01    1.26938600000E-02   -2.49460000000E-06    1.89321300000E-10    0.
                                1.20924970573E+03    2.14770000000E+04    3.86000000000E+02
N2         2.99994817506E+00    4.39234000000E+01    1.22250100000E-02   -2.37900500000E-06    1.79832200000E-10    0.
                                1.13916134896E+03    0.                   3.80000000000E+02
OH         4.96489085787E-10    4.24179200000E+01    1.15684700000E-02   -2.22665900000E-06    1.68915500000E-10    0.
                                1.18351754427E+03    3.56000000000E+03    4.13000000000E+02
CH4        3.61824388775E-07    3.87568600000E+01    2.36401300000E-02   -3.70795700000E-06    2.47071400000E-10    0.
                                1.04242791146E+03   -1.60000000000E+04    5.28000000000E+02
SOL C      1.48985.38705E+00   -2.46151900000E-01    7.17985500000E-03   -1.29755000000E-06    9.34599500000E-11    0.
                               -2.58204389323E+02    0.                   0.
```

```
 THE BKW HUGONIOT FOR THE DETONATION PRODUCTS OF
 RDX       CYCLOTRIMETHYLENE TRINITRAMINE


PRESSURE =  5.00000000000E-01 VOLUME =  3.68557080033E-01 TEMPERATURE =  2.86379819612E+03
SHOCK VELOCITY =  9.08433266937E-01 PARTICLE VELOCITY = 3.05236661417E-01 UNITS ARE MBARS,CC/GM, DEG K, AND CM/MICROSECOND


 SPECIE   NO OF MOLES
H2O      2.99998545678E+00
H2       1.75209929177E-06
O2       2.99312928467E-05
CO2      1.49307822159E+00
CO       1.34952144336E-02
NH3      8.46270471251E-06
H        1.92957891433E-09
NO       3.03021745638E-04
N2       2.99984425777E+00
OH       1.46899774007E-09
CH4      4.76844982552E-08
SOL C    1.49342651630E+00


PRESSURE =  4.50000000000E-01 VOLUME =  3.81506073891E-01 TEMPERATURE =  2.75345203113E+03
SHOCK VELOCITY =  8.93299111665E-01 PARTICLE VELOCITY = 2.79650072618E-01 UNITS ARE MBARS,CC/GM, DEG K, AND CM/MICROSECCND


 SPECIE   NO OF MOLES
H2O      2.99998078763E+00
H2       2.52522105824E-06
O2       1.35656309186E-05
CO2      1.49266608115E+00
CO       1.44776503827E-02
NH3      1.10252722769E-05
H        4.65427904492E-10
NO       1.82267984964E-04
N2       2.99990335337E+00
OH       4.02414879069E-10
CH4      7.44019661677E-08
SOL C    1.49285619407E+00


PRESSURE =  4.00000000000E-01 VOLUME =  3.96585070658E-01 TEMPERATURE =  2.66222674513E+03
SHOCK VELOCITY =  8.81249123861E-01 PARTICLE VELOCITY = 2.52128721802E-01 UNITS ARE MBARS,CC/GM, DEG K, AND CM/MICROSECOND


 SPECIE   NO OF MOLES
H2O      2.99997078656E+00
H2       4.31472749893E-06
O2       6.27020787340E-06
CO2      1.49155216049E+00
CO       1.67981726650E-02
NH3      1.64097066746E-05
H        4.85313590782E-10
NO       1.14178952130E-04
N2       2.99993470567E+00
OH       4.31442574033E-10
CH4      1.41845903046E-07
SOL C    1.49164952500E+00


PRESSURE =  3.50000000000E-01 VOLUME =  4.14600769335E-01 TEMPERATURE =  2.59153062904E+03
SHOCK VELOCITY =  8.75429108468E-01 PARTICLE VELOCITY = 2.22112965089E-01 UNITS ARE MBARS,CC/GM, DEG K, AND CM/MICROSECOND


 SPECIE   NO OF MOLES
H2O      2.99994794445E+00
H2       8.93854167661E-06
O2       3.02430422377E-06
CO2      1.48927526506E+00
CO       2.14194943420E-02
NH3      2.82929973680E-05
H        5.35071178956E-10
NO       7.59819829510E-05
N2       2.99994786251E+00
OH       4.91167677137E-10
CH4      3.38498479404E-07
SOL C    1.48930490210E+00


PRESSURE =  3.00000000000E-01 VOLUME =  4.36835280098E-01 TEMPERATURE =  2.54370083879E+03
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 SPECIE   NO OF MOLES
H20       2.99988911914E+00
H2        2.29785316955E-05
O2        1.56725927136E-06
CO2       1.48474001089E+00
CO        3.05726923301E-02
NH3       5.72203253117E-05
H         6.25410207065E-10
NO        5.50316386149E-05
N2        2.99994387402E+00
OH        5.92628655103E-10
CH4       1.03561532141E-06
SOL C     1.48468626116E+00


PRESSURE =  2.50000000000E-01 VOLUME =  4.65492054077E-01 TEMPERATURE =  2.52225168612E+03


 SPECIE   NO OF MOLES
H20       2.99971100941E+00
H2        7.50244687743E-05
O2        9.02931899893E-07
CO2       1.47517781751E+00
CO        4.9[illegible]68[illegible]2398E-02
NH3       1.37051753754E-04
H         8.27406842919E-08
NO        4.45955588281E-05
N2        2.99990917635E+00
OH        7.29569073208E-08
CH4       4.15533367510E-06
SOL C     1.47494114591E+00


PRESSURE =  2.00000000000E-01 VOLUME =  5.04768663355E-01 TEMPERATURE =  2.53174658206E+03


 SPECIE   NO OF MOLES
H20       2.99905152153E+00
H2        3.17954574076E-04
O2        5.96579368401E-07
CO2       1.45298361590E+00
CO        9.49383020624E-02
NH3       3.90415086854E-04
H         2.98714838215E-07
NO        4.14696690567E-05
N2        2.99978405762E+00
OH        2.81781678836E-07
CH4       2.23055089619E-05
SOL C     1.45205577653E+00


PRESSURE =  1.50000000000E-01 VOLUME =  5.63965128855E-01 TEMPERATURE =  2.57565620937E+03


 SPECIE   NO OF MOLES
H20       2.99591143015E+00
H2        1.78372116349E-03
O2        4.50998348192E-07
CO2       1.39491864343E+00
CO        2.14204557745E-01
NH3       1.31814880621E-03
H         1.58990809610E-06
NO        4.43242202272E-05
N2        2.99931876349E+00
OH        1.49903363334E-06
CH4       1.63040501926E-04
SOL C     1.39071375833E+00


PRESSURE =  1.00000000000E-01 VOLUME =  6.69390292687E-01 TEMPERATURE =  2.64623490861E+03


 SPECIE   NO OF MOLES
H20       2.97504092530E+00
H2        1.36668866707E-02
O2        3.37533931589E-07
CO2       1.22857497519E+00
CO        5.67748710634E-01
NH3       5.26496255947E-03
H         1.24983060644E-05
NO        4.96035227474E-05
N2        2.99734271696E+00
OH        1.01351058357E-05
CH4       1.69171374366E-03
SOL C     1.20198460044E+00
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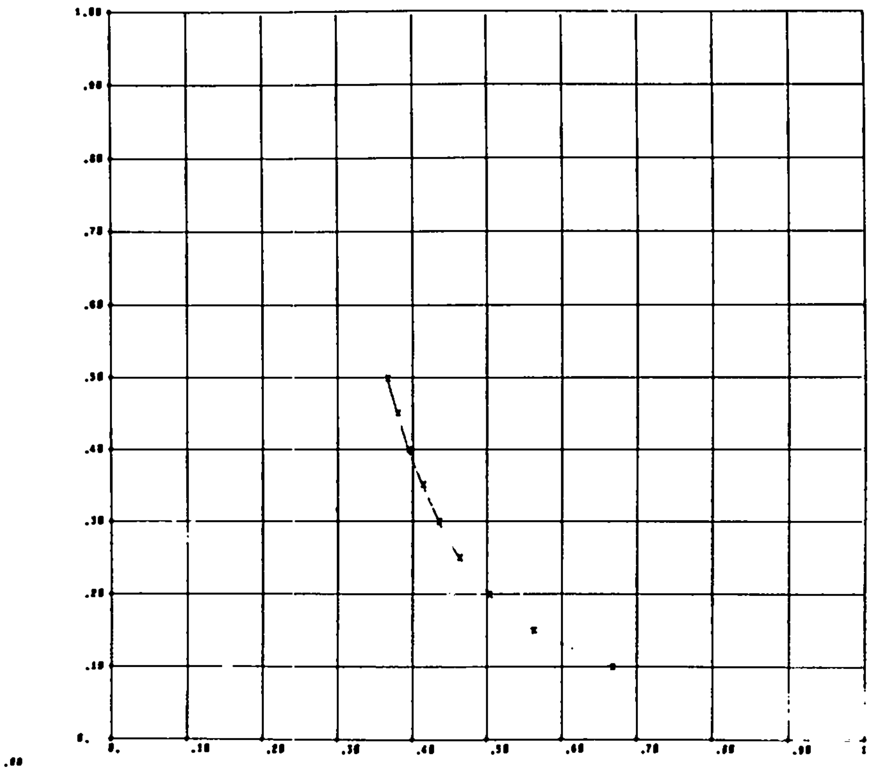
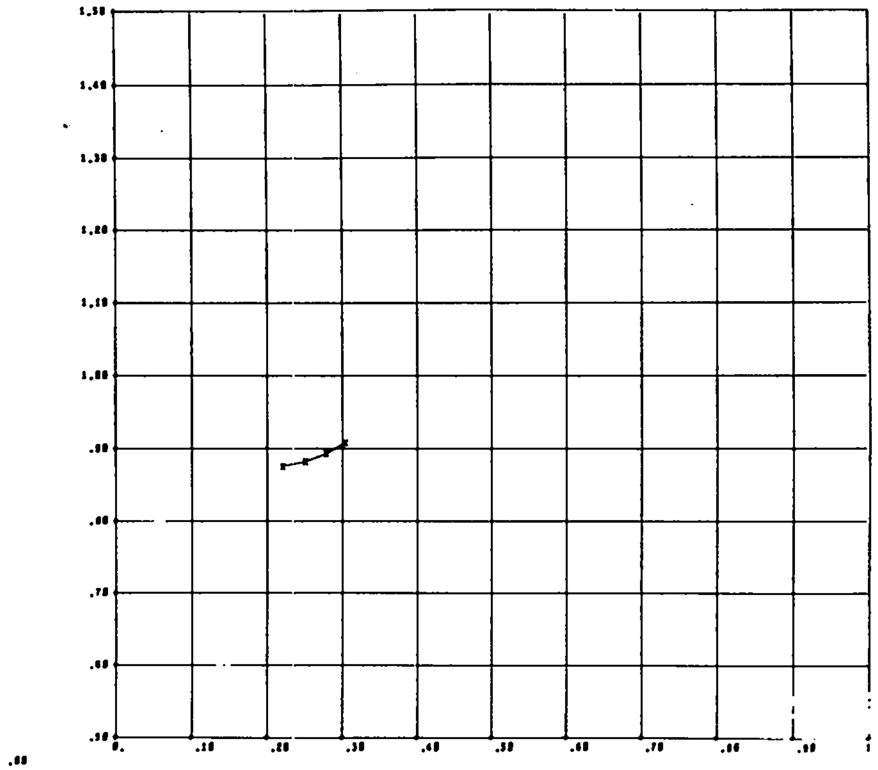


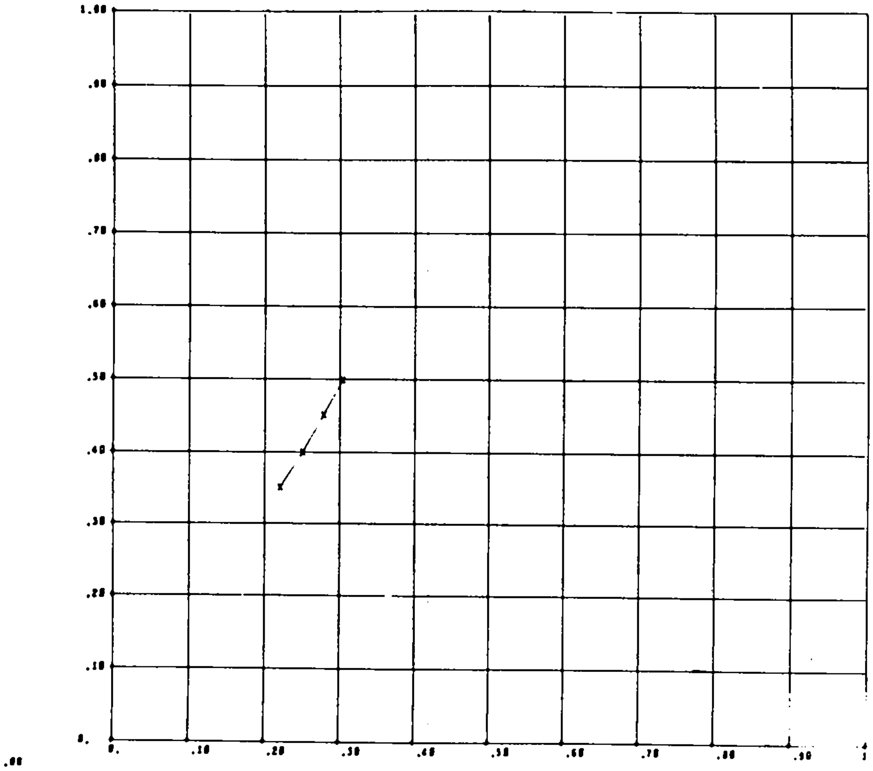
RDX CYCLOTRIMETHYLENE TRINITRAMINE

PRESSURE (MBARS) - VOLUME (CC/GM) HUGONIOT



RDX CYCLOTRIMETHYLENE TRINITRAMINE

SHOCK VELOCITY - PARTICLE VELOCITY HUGONIOT



RDX CYCLOTRIMETHYLENE TRINITRAMINE

PRESSURE (MBARS) - PARTICLE VELOCITY (CM/USEC) HUGONIOT

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A BKW ISENTROPE THRU BKW CJ PRESSURE FOR
RDX       CYCLOTRIMETHYLENE TRINITRAMINE


LN(P)= -3.49297740731E+00   -2.54806028626E+00LNV   2.56284384201E-01LNV*2  9.74735285967E-03LNV*3 -9.36281889664E-03LNV*4

LN(T)=  7.41443241083E+00   -4.90817152634E-01LNV   3.75181959834E-02LNV*2  2.84869451321E-02LNV*3 -9.96133737672E-03LNV*4

LN(E)= -1.60502412233E+00    5.19208252102E-01LNP   6.59353610896E-02LNP*2  4.07879169323E-03LNP*3  9.83423378158E-05LNP*4

THE CONSTANT ADDED TO ENERGIES WAS  1.00000000000E-01

    PRESSURE (MBARS)     VOLUME (CC/GM)       TEMPERATURE (DEG K)  ENERGY+C (MB-CC/GM)  GAMMA (-DLNP/DLNV)   PARTICLE VELOCITY
    3.46662648781E-01    4.15935350982E-01    2.58759366556E+03    1.24200627104E-01    2.94991700019E+00    2.20082528743E-01
    2.42663854147E-01    4.69093987956E-01    2.44025410622E+03    1.08763295438E-01    2.90305348576E+00    2.93278938450E-01
    1.69864697903E-01    5.29965625166E-01    2.29059666043E+03    9.63895994894E-02    2.85213737241E+00    3.58965587946E-01
    1.18905288532E-01    6.00189284098E-01    2.14384498360E+03    8.63993698681E-02    2.79712834225E+00    4.18182027779E-01
    8.32337019724E-02    6.81803562866E-01    2.00434562728E+03    7.83093065606E-02    2.73798722098E+00    4.71815131800E-01
    5.82635913807E-02    7.77028859144E-01    1.87044783371E+03    7.16597794967E-02    2.67490765179E+0J    5.20429991637E-01
    4.07845139665E-02    8.88907438901E-01    1.74509810113E+03    6.61902223966E-02    2.60795481141E+00    5.64653101227E-01
    2.85491597765E-02    1.02113784639E+00    1.62857115419E+03    6.16638941052E-02    2.53732615598E+00    6.04969694274E-01
    1.99844118436E-02    1.17838616759E+00    1.52077981649E+03    5.78953120500E-02    2.46330197961E+00    6.41805711625E-01
    1.39890882905E-02    1.36695791246E+00    1.42249053138E+03    5.47622930232E-02    2.38612407116E+00    6.75597797322E-01
    9.79236180335E-03    1.59385614894E+00    1.33126090094E+03    5.21076951821E-02    2.30656211859E+00    7.06571279570E-01
    6.85465326234E-03    1.86879462348E+00    1.24721284584E+03    4.98564394379E-02    2.22527636309E+00    7.35051238503E-01
    4.79825728364E-03    2.20386399502E+00    1.16962429208E+03    4.79361788042E-02    2.14324065525E+00    7.61291260795E-01
    3.35878009855E-03    2.61447561825E+00    1.09769295739E+03    4.62891331058E-02    2.06168176994E+00    7.85520933819E-01
    2.35114606898E-03    3.12037929395E+00    1.03056914280E+03    4.48687813973E-02    1.98209640991E+00    8.07952301967E-01
    1.64580224829E-03    3.74699459602E+00    9.67409628208E+02    4.36374387357E-02    1.90627163434E+00    8.28782539811E-01
    1.15206157380E-03    4.52712000911E+00    9.07437880573E+02    4.25644767890E-02    1.83630876977E+00    8.48194083404E-01
    8.06443101661E-04    5.50024262141E+00    8.49288991539E+02    4.16149056999E-02    1.77479290456E+00    8.66307651573E-01
    5.64510171163E-04    6.72682919669E+00    7.94080445607E+02    4.07923523906E-02    1.72414737918E+00    8.83378800275E-01
    3.951571198'4E-04    8.27415256663E+00    7.40475883596E+02    4.00656452946E-02    1.68771205200E+00    8.99476598168E-01
    2.76609983870E-04    1.02313668969E+01    6.88201867397E+02    3.94216420729E-02    1.66889738083E+00    9.14708556278E-01
    1.93626988709E-04    1.27103240328E+01    6.37068895323E+02    3.88501274872E-02    1.67129629277E+00    9.29155085569E-01
    1.35538892096E-04    1.58482086738E+01    5.86929621037E+02    3.83432881871E-02    1.69850373407E+00    9.42862453873E-01
    3.98662046098E-01    3.96885356962E-01    2.64297698676E+03    1.31281189881E-01    2.96720440286E+00    0.
    4.58461353013E-01    3.78694889350E-01    2.69633703138E+03    1.39060223226E-01    2.98391886698E+00    0.
    5.27230555965E-01    3.61228541397E-01    2.74697021400E+03    1.47650805025E-01    3.00012646195E+00    0.
    6.06315139360E-01    3.44202840737E-01    2.79504209255E+03    1.57283774060E-01    3.01603533850E+00    0.
    6.97262410264E-01    3.26300934698E-01    2.84834367405E+03    1.68947916544E-01    3.03282442827E+00    0.
    8.01851771804E-01    3.11225320419E-01    2.88721210089E+03    1.80250775357E-01    3.04695587055E+00    0.
    9.22129537574E-01    2.97898690227E-J1    2.90313821785E+03    1.91682860924E-01    3.05939136224E+00    0.


THE ISENTROPE STATE VARIABLES AS COMPUTED FROM THE LEAST SQUARES FIT

    BKW PRESSURE         FIT PRESSURE         BKW TEMPERATURE      FIT TEMPERATURE      BKW ENERGY + C       FIT ENERGY
    3.46662648781E-01    3.42097052513E-01    2.58759366556E+03    2.56248322413E+03    1.24200627104E-01    1.24207887420E-01
    2.42663854147E-01    2.40586891593E-01    2.44025410622E+03    2.42874182890E+03    1.08763295438E-01    1.08692586884E-01
    1.69864697903E-01    1.69348084478E-01    2.29059666043E+03    2.28081441187E+03    9.63895994894E-02    9.63283656878E-02
    1.18905288532E-01    1.19157824052E-01    2.14384498360E+03    2.14374764316E+03    8.63993698681E-02    8.63788985581E-02
    8.32337019724E-02    8.37275002576E-02    2.00434562728E+03    2.01044426539E+03    7.83093065606E-02    7.82990742685E-02
    5.82635913807E-02    5.87748147611E-02    1.87044783371E+03    1.88210244389E+03    7.16597794967E-02    7.16866682178E-02
    4.07845139665E-02    4.11975746634E-02    1.74509810113E+03    1.75935749854E+03    6.61902223966E-02    6.62354393554E-02
    2.85491597765E-02    2.88350291672E-02    1.62857115419E+03    1.64284109578E+03    6.16638941052E-02    6.17122099676E-02
    1.99844118436E-02    2.01552733611E-02    1.52077981649E+03    1.53302234751E+03    5.78953120500E-02    5.79368955460E-02
    1.39890882905E-02    1.40628357727E-02    1.42249053138E+03    1.43002884815E+03    5.47622930232E-02    5.47689247219E-02
    9.79236180335E-03    9.80820985465E-03    1.33126090094E+03    1.33435447118E+03    5.21076951821E-02    5.20974059455E-02
    6.85465326234E-03    6.83905135458E-03    1.24721284584E+03    1.24593144496E+03    4.98564394379E-02    4.98339695218E-02
    4.79825728364E-03    4.77055131434E-03    1.16962429208E+03    1.16465802206E+03    4.79361788042E-02    4.79075057165E-02
    3.35878009855E-03    3.33112793191E-03    1.09769295739E+03    1.09025671132E+03    4.62891331058E-02    4.62602652588E-02
    2.35114606898E-03    2.32969823481E-03    1.03056914280E+03    1.02225131116E+03    4.48687813973E-02    4.48449488752E-02
    1.64580224829E-03    1.63242269053E-03    9.67409628208E+02    9.59951953587E+02    4.36374387357E-02    4.36225217712E-02
    1.15206157380E-03    1.14601521241E-03    9.07437880573E+02    9.02445091382E+02    4.25644767890E-02    4.25605642298E-02
    8.06443101661E-04    8.06481025547E-04    8.49288991539E+02    8.48723971171E+02    4.16149056999E-02    4.16320218042E-02
    5.64510171163E-04    5.67208877661E-04    7.94080445607E+02    7.97103072372E+02    4.07923523906E-02    4.08142553807E-02
    3.95157119814E-04    3.98550888842E-04    7.40475883596E+02    7.46188169792E+02    4.00656452946E-02    4.00883167624E-02
    2.76609983870E-04    2.79176948071E-04    6.88201867397E+02    6.94281268932E+02    3.94216420729E-02    3.94383963874E-02
    1.93626988709E-04    1.94401041282E-04    6.37068895323E+02    6.39721859514E+02    3.88501274872E-02    3.88513981900E-02
    1.35538892096E-04    1.34107925500E-04    5.86929621037E+02    5.81168656999E+02    3.83432881871E-02    3.83166144129E-02
    3.98662046098E-01    3.92996643917E-01    2.64297698676E+03    2.61833667923E+03    1.31281189881E-01    1.31355575861E-01
    4.58461353013E-01    4.31873509384E-01    2.69633703138E+03    2.67436057532E+03    1.39060223226E-01    1.39214475716E-01
    5.27230555965E-01    5.20449318751E-01    2.74697021400E+03    2.73072043565E+03    1.47650805025E-01    1.47871059180E-01
    6.06315139360E-01    6.01799600712E-01    2.79504209255E+03    2.78813873069E+03    1.57283774060E-01    1.57424348318E-01
    6.97262410264E-01    7.07308127395E-01    2.84834367405E+03    2.85117739800E+03    1.68947916544E-01    1.67987890936E-01
    8.01851771804E-01    8.16694293650E-01    2.88721210089E+03    2.90635752274E+03    1.80250775357E-01    1.79692195604E-01
    9.22129537574F-01    9.33448003657E-01    2.90313821785E+03    2.95666916073E+03    1.91682860924E-01    1.92687622960E-01
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  THE ISENTROPE PRESSURE AND COMPOSITION OF DETONATION PRODUCTS
H2O    H2     O2      CO2    CO     NH3    H       NO     N2      OH      CH4     SOL C
    3.46662648781E-01     2,99994556597E+00     9,45374836410E-06     2,88697880055E-06     1,48906096240E+00     2,18525889737E-02
    2.95040751845E-05     5,39687882169E-10     7,41458034518E-05     2,99994817506E+00     4,96489084344E-10     3,61824334079E-07
    1,48908698680E+00
    2,42663854147E-01     2,99976043518E+00     6,09941217255E-05     5,21332382729E-07     1,47916778172E+00     4,18738838230E-02
    1,14756429427E-04     5,07547218678E-08     2,90291441216E-05     2,99992810721E+00     4,57586668323E-08     3,19390071298E-06
    1,47895514056E+00
    1.69864697903E-01     2,99920373220E+00     2,72662825546E-04     8,99891545553E-08     1,46611943938E+00     6,85467598778E-02
    3,25021707223E-04     9,89322588324E-08     1,03468345323E-05     2,99983231573E+00     1,02356137151E-07     1,79858850558E-05
    1,46531581486E+00
    1,18905288532E-01     2,99780389432E+00     9,31963083371E-04     5,08137252220E-10     1,45103509976E+00     1,00122417136E-01
    7,40901472975E-04     1,43972287333E-07     3,32853093012E-06     2,99962788500E+00     1,59488371639E-07     7,63193292440E-05
    1,44876616378E+00
    8,32337018724E-02     2,99468942998E+00     2,60381197673E-03     2,83910839781E-10     1,43550724713E+00     1,34294911952E-01
    1,44688203107E-03     1,66675128560E-07     9,76633830323E-07     2,99927607067E+00     1,86612883497E-07     2,68129177082E-04
    1,42992971174E+00
    5,82635913807E-02     2,98858961284E+00     6,08951295615E-03     1,20583081871E-10     1,42287642160E+00     1,65657121393E-01
    2,47731299659E-03     1,53702059064E-07     2,55690415222E-07     2,99876121566E+00     1,66621601184E-07     8,02372271080E-04
    1,41066408473E+00
    4,07845139665E-02     2,97766739078E+00     1,23606457337E-02     2,88706525368E-11     1,4'568948004E+00     1,90955468223E-01
    3,82556219651E-03     1,17939826750E-07     6,09579170639E-08     2,99808718842E+00     1,19901545931E-07     2,11675063345E-03
    1,39123930111E+00
    2,85491597765E-02     2,95976403777E+00     2,21834839558E-02     1,00000000000E-11     1,41667736755E+00     2,06881155101E-01
    5,39766330350E-03     7,66791362799E-08     4,99134882360E-10     2,99730116810E+00     7,15431657550E-08     4,97795460571E-03
    1,37146352275E+00
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    1,07680829112E+00
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    1,50016811578E+00
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    4,99358206855E-10     3,36368965094E-11     1,18894690242E-03     2,99940552630E+00     1,42546826648E-11     1,00000000000E-11
    1,50174263411E+00
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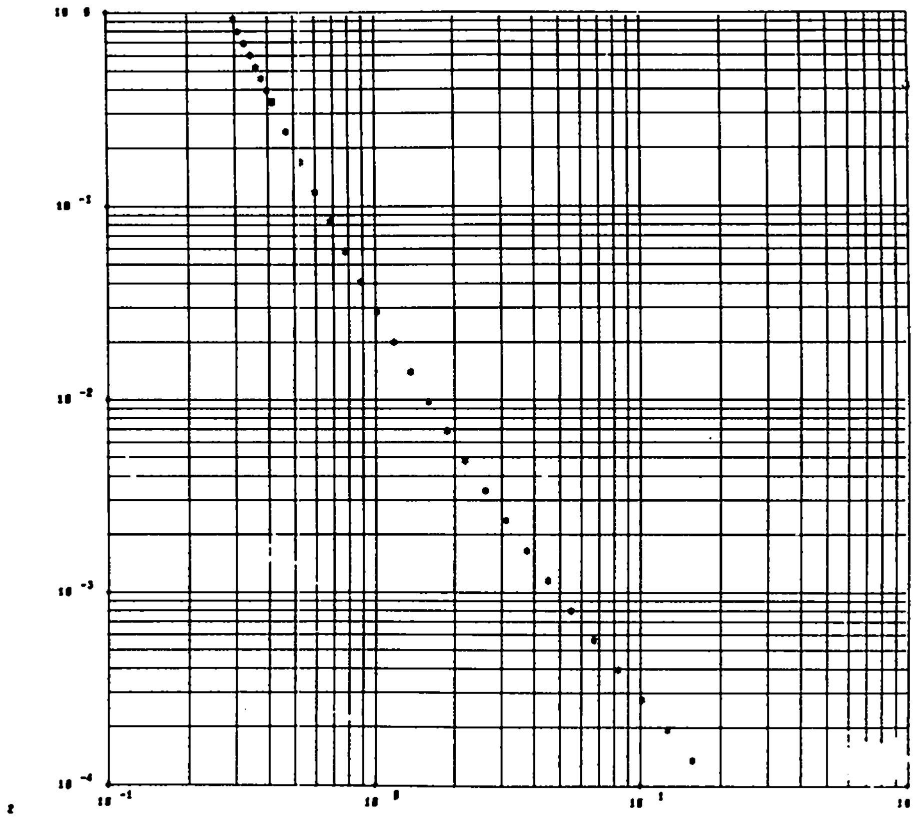
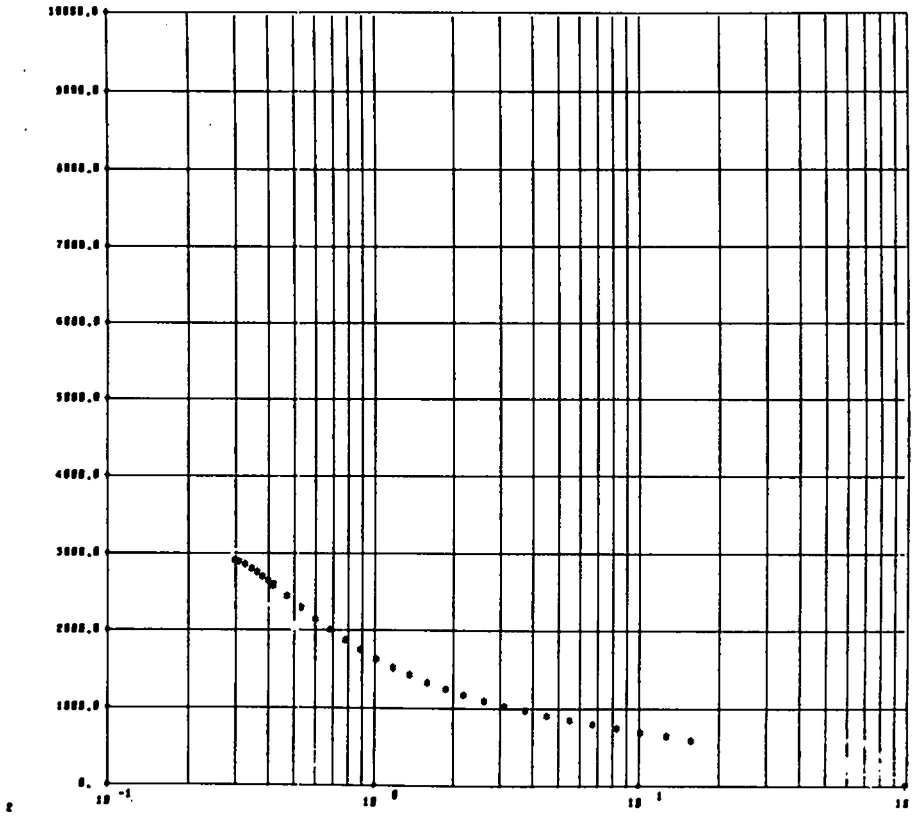


RDX CYCLOTRIMETHYLENE TRINITRAMINE
PRESSURE-VOLUME ISENTROPE THRU THE C-J VALUE



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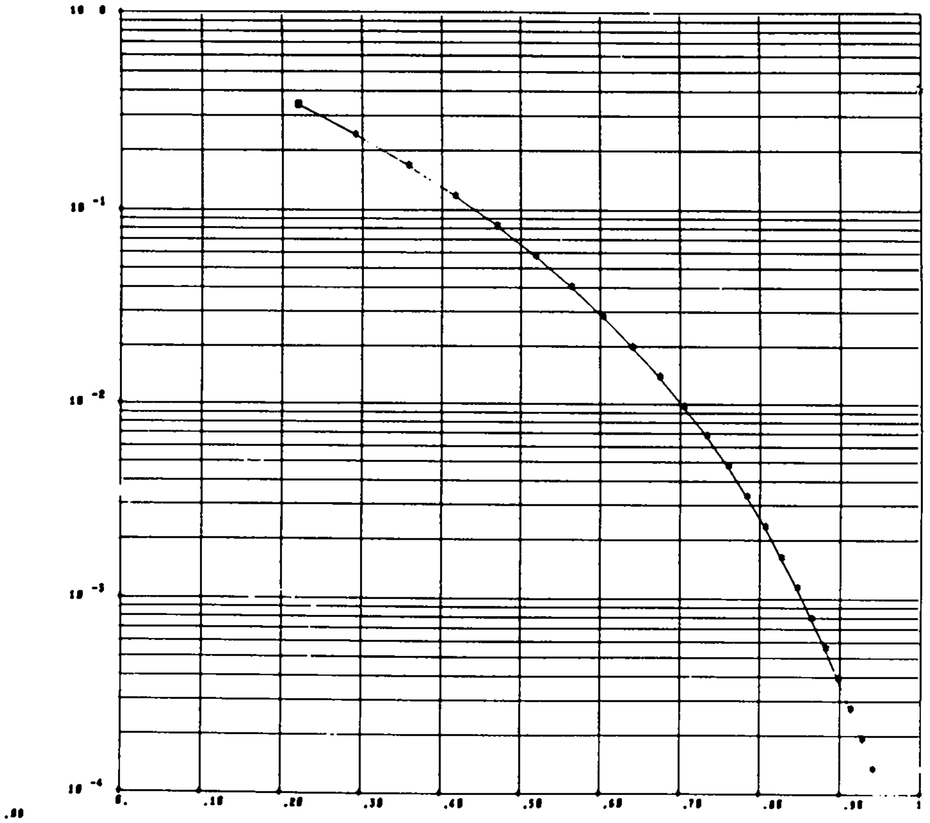
TEMPERATURE -VOLUME ISENTROPE THRU THE C-J VALUE



RDX CYCLOTRIMETHYLENE TRINITRAMINE
PRESSURE -PARTICLE VELOCITY ISENTROPE

V. FORTRAN BKW CODING FORMULAS. Stretch BKW consists of numerous subroutines, both self-sufficient and dependent. The self-sufficient subroutines are described in Appendix I.

The dependent subroutines form the main body of the code under the control of a master control routine which performs only the operations requested by the input. A dependent subroutine uses the results of other dependent subroutines and assumes that certain sequences of operations have preceded it.

System I. Given P and T, compute V_g. Coded as SUBROUTINE SYS1(IND).

1. $\sum_{i=1}^{N} X_i = \bar{X}$.

2. $Z = K \sum_{i=1}^{N} \frac{X_i}{\bar{X}} k_i$.

3. Linear feedback on V_g. (See Appendix IB for description of routine.) (VBOS) = Initial guess = 15, Ratio = 1.1, Error = 1×10^{-8}.

   a. $W = \frac{Z}{V_g(T+\theta)^{\alpha}}$

   b. $1 + We^{\beta W} = F_{(x)}$.

   c. $0 = F_{(x)} - \frac{PV_g}{R_2T}$.

4. Find F_i^* for i = 1to N.

   a. Call thermodynamic function subroutine for $(F - HO/T)_i$ for i = 1 to NT.

   b. Form

$$F_i^* = \left(\frac{F-HO}{R_iT}\right)_i + \frac{(\Delta H_f^o)_i}{R_1T} + \ln(R_4 \cdot P)$$
$$- \left[\ln F_{(x)} - \left(\frac{e^{\beta W}-1}{\beta}\right) - Kk_i \frac{F_{(x)}-1}{Z}\right].$$

5. Find $(V_s)_i$ and $(G^*)_i$ for i = N+1 to NT.

   a. Call Cowan solid equation of state subroutine for V_s and then F_s'.

$$(G^*)_i = \left(\frac{F-HO}{R_1T}\right)_i + \frac{(\Delta H_f^o)_i}{R_1T} + \frac{F_s'}{R_2T}.$$

6. Enter equilibrium subroutine to compute new X_i.

7. Test for convergence.

$$\sum_{i=1}^{NT} |Y_i - X_i| < 2 \times 10^{-5} \text{ (EXITME)}.$$

If not converged, return to step 1.

System II. Given P, T and V, calculate E. Coded as SUBROUTINE SYS2. Assumes System I has been performed.

1. $E'_g = R_1 T \left(\alpha T \frac{F_{(x)}-1}{T+\theta} \right).$

2. $E_g = \left\{ \sum_{i=1}^{N} \frac{X_i}{\bar{X}} \left[(H-HO)_i - R_1 T + (\Delta H_f^o)_i \right] \right\} + E'_g,$

   where $(H-HO)_i$ was obtained using the thermodynamic function subroutine for $i = 1$ to NT.

3. $(E_s)_i = (H-HO)_i + (\Delta H_f^o)_i + R_3 E'_s$

   for $i = N + 1$ to NT, where E'_s was obtained from the Cowan solid equation of state subroutine.

4. $E_{Total} = \bar{X}_g E_g + \sum_{i=N+1}^{NT} X_i (E_s)_i.$

5. $V_{Total} = \bar{X}_g V_g + \sum_{i=N+1}^{NT} X_i (\bar{V}_s)_i (MOLWT)_i.$

6. $VPG = (V_{Total})/(AMOLWT).$

System II A. Given a P, compute Hugoniot temperature. Coded as SUBROUTINE SYS2A(IND).

1. Linear feedback on T.

   (HUGBOS) = Initial guess = 3000°K, RATIO = 1.1, ERROR = 1×10^{-6}.

   $$0 = (1 \times 10^{-5}) \left[E_{Total} - E_o - 1/2(P+P_o)(V'_o - VPG)(R_3) \times (AMOLWT) \right].$$

   $P_o = (PO) = 1 \times 10^{-6}.$

Enter System I and II to find the necessary values. 1×10^{-5} is SCALF, a convenient scaling constant.

System III. Find the C-J Values. Coded as SUBROUTINE SYS3(IND).

1. (CJBOS) = $P_{guessed} = 0.15 + 0.25(\rho_o - 1).$

   0.15 is in APGCJ, and 0.25 in BPGCJ.
   Ratio = 0.8, ERROR = 1×10^{-6}.

2. Use minimum of a parabola subroutine for

   $$D = V'_o \left(\frac{P-P_o}{V'_o - VPG} \right)^{\frac{1}{2}}$$

   Use System II A to find the necessary values.

3. $\gamma_{CJ} = \frac{\rho_o D^2}{P_{CJ}} - 1.$

4. $U_{CJ} = \left[P_{CJ} (V'_o - VPG) \right]^{\frac{1}{2}}.$

System IV. Given P, T and V, calculate S. Coded as SUBROUTINE SYS4. Assumes System I has been performed.

1. $$S'_g = -R_1 \left[\sum_{i=1}^{N} \left(\frac{X_i}{\bar{X}} \ln \frac{X_i}{\bar{X}} \right) + \ln (R_4 \cdot P) \right] + R_1 \left\{ \ln F_{(X)} - \left(\frac{e^{\beta w} - 1}{\beta} \right) + \frac{\alpha T \left[F_{(X)} - 1 \right]}{(T+\theta)} \right\}.$$

2. $S_g = \sum_{i=1}^{N} \frac{X_i}{\bar{X}} S_i^o + S'_g,$

   where S_i^o for $i = 1$ to NT was obtained from thermodynamic function subroutine.

3. $(S_s)_i = S_i^o + \frac{R_3 (S'_s)_i}{R_5}$, for $i = N+1$ to NT,

   where S'_s was obtained from the Cowan solid equation of state routine.

4. $S_{Total} = \bar{X}_g S_g + \sum_{i=N+1}^{NT} X_i (S_s)_i$.

System IV A. To compute the CJ isentrope for the CJ pressure. Coded as SUBROUTINE SYS4A(IND).

1. From the CJ pressure, find the Hugoniot temperature and energy using System II A, and the CJ entropy using System IV.

2. From the CJ point, first decrease P by multiples of DECIP = 0.175 until you reach AMINP (1×10^{-4}). Then increase P_{CJ} by multiples of AINCP (1.15) until you reach AMAXP (1.0).

3. Find the isentrope value by using linear feedback on T and the equation

   $S_{Total} - S_{CJ} = 0$ using System IV.

   ASBOS = Initial guess = CJ T, Ratio = 0.9, Error = 0.1 for $P < P_{CJ}$.

ASBOSH = Initial guess = CJ T, Ratio = 1.1, Error = 0.1 for $P > P_{CJ}$.

4. Maximum number of isentrope points is 100.
5. When an isentrope point is found, System II is used to find the energy.

$$E' = (E_{Total} - E_o)/[(R_3)(AMOLWT)] + CPRIME.$$

E' units are Mbar - cc/g.

CPRIME = 0.1 is a constant to keep E positive.

6. Fits of $\ln P = f(\ln V) = A' + B'\ln V + C'\ln V^2 + D'\ln V^3 + E'\ln V^4$,

$$\ln T = f(\ln V),$$
$$\ln E' = f(\ln P),$$

were obtained using PFTS, a Los Alamos Scientific Laboratory least-squares subroutine.

7. $\gamma = -\frac{(d\ln P)}{(d\ln V)}$ from the fit of $\ln P = f(\ln V)$.

8. Particle velocity

$$U_p = (U_p)_{CJ} + \int_{V_{CJ}}^{V} (-\frac{dP}{dV})^{\frac{1}{2}} dV,$$

accomplished using Simpson's rule and finding dP/dV from the fit by

$-\frac{dP}{dV} = \frac{-P}{V}\frac{d\ln P}{d\ln V}$ for 100 increments between each isentrope point.

Simpson's rule is

$$S = \frac{\Delta V}{3}(Y_1 + 4Y_2 + 2Y_3 + 4Y_{n-1} + \ . \ . \ . \ Y_n),$$

where n = 101, ΔV is volume increment, and Y is $(-\frac{dP}{dV})^{\frac{1}{2}}$.

System V. Compute Hugoniot curve. Coded as SUBROUTINE SYS5(IND). Using System II A to compute the necessary values, find P by

1. P = AMHUGP - (n)(DELP) until it is less than DELP where n = 0 for 1st calculation, 1 for 2nd, etc., P = 0.5 - n(0.05).
2. Max number of Hugoniot points is 20.
3. $U_s = V_o' \left(\frac{P}{V_o' - VPG}\right)^{\frac{1}{2}}$ computed if $P > P_{CJ}$.
4. $U_p = (U_p)_{CJ} + (P - P_{CJ})(V_{CJ} - VPG)$ computed if $P > P_{CJ}$.

Note: VBOS(1) is set equal to VBOS 2, and HUGBOS(1) is set equal to HUGBOS 2 each time the previous history of the problem can result in an undesirable result left in VBOS(1) and HUGBOS(1).

VI. CONSTANT IDENTITY NUMBERS FOR THE CONSTANTS.

Identity Value	Name of Constant	Value in Code
1	VBOS(1)	15
2	VBOS(2)	1.1
3	VBOS(3)	1.0×10^{-8}
4	EXITME	2×10^{-5}
5	HUGBOS(1)	3000
6	HUGBOS(2)	1.1
7	HUGBOS(3)	1.0×10^{-6}
8	PO	1.0×10^{-6}
9	CJBOS(2)	0.8
10	CJBOS(3)	1.0×10^{-6}
11	APGCJ	0.15
12	BPGCJ	0.25
13	AMHUGP	0.5
14	DELP	0.05
15	CPRIME	0.1
16	DECIP	0.75
17	AMINP	1×10^{-4}
18	AINCP	1.15
19	AMAXP	1.0
20	ABOS(2)	0.9
21	ABOS(3)	0.1
22	ABOSH(2)	1.1
23	ABOSH(3)	0.1
24	VBOS2	15
25	HUGBOS2	3000
26	AMAXE	1.0×10^{-8}
27	AMINX	1.0×10^{-11}
28	AMINY	1.0×10^{-7}
29	TX(2)	1.1
30	TX(3)	1.0×10^{-9}

For a few problems it has been found necessary to change 5, 9, 12, 26, and 27 to obtain convergence. Another use of this feature is to change the range and intervals of the various calculations. Once a constant has been changed, it will be changed for further explosive calculations unless the new set of input restores the constant to its original value.

APPENDIX I

SELF-SUFFICIENT FORTRAN SUBROUTINES

A. Equilibrium Subroutine. This subroutine computes the equilibrium composition for a system of 10 elements, 20 gaseous species, and five solids. Only one of the solids is permitted to disappear. The subroutine is based on a modified version of the minimization of free energy technique described by White, Johnson, and Dantzig.[6]

The Formulas

$$\bar{X} = \sum_{i=1}^{N} X_i \qquad \bar{Y} = \sum_{i=1}^{N} Y_i$$

$$f_i(y) = F_i^* + \ln \frac{y_i}{\bar{y}} \quad \text{for } i = 1 \text{ to } N$$

$$G_i(y) = G_i^* \quad \text{for } i = N + 1 \text{ to NT}$$

To form [A]X = [B], the equations are

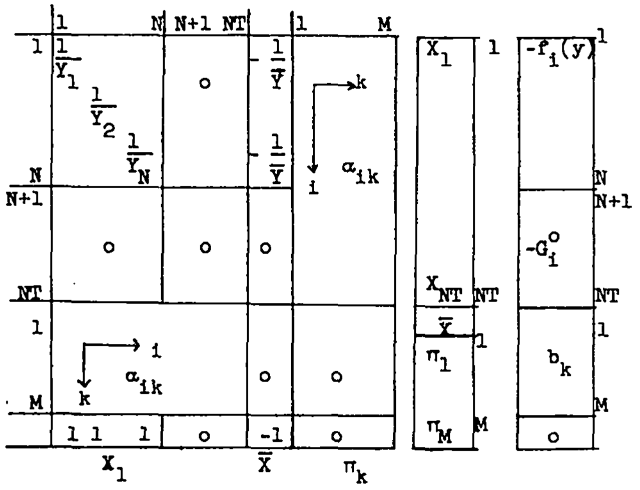
$$\frac{X_i}{Y_i} - \frac{\bar{X}}{\bar{Y}} + \sum_{k=1}^{M} \pi_k \alpha_{ik} = -f_i(y) \quad \text{for } i = 1 \text{ to } N$$

$$\sum_{k=1}^{M} \pi_k \alpha_{ik} = -G_i(y) \quad \text{for } i = n + 1 \text{ to NT}$$

$$\sum_{k=1}^{M} \alpha_{ik} X_i = b_k \quad \text{for } i = 1 \text{ to NT}$$

$$\sum_{i=1}^{N} X_i - \bar{X} = 0$$

The Matrix [A]X = [B]



The matrix is solved with the Los Alamos Scientific Laboratory subroutine LSS (Linear System Solver).

The Constraints

1. The initial Y_i may not be smaller than 1×10^{-7} (AMINY).
2. The X_i for i = 1to N may not be smaller than 1×10^{-11} (AMINX).
3. The X_i for i = N + 1to NT may not be negative. If one is negative and it is the last solid, it is eliminated. If it is not the last solid, then an error return occurs.
4. The system has converged when
$$\sum_{i=1}^{NT} |Y_i - X_i| < 1 \times 10^{-8} \text{ (AMAXE)}.$$
5. Otherwise X_i for i = 1 to NTto Y for i = 1 to NT and resolve.

If the equilibrium scheme is not part of an outside loop, constraint 4 must be satisfied before constraint 3 is tested or a solid may disappear in error. With an outside loop, such as in BKW, the error corrects itself and a considerable saving in machine time is achieved for systems in which one solid is supposed to disappear.

Programming Instructions

CALL EQUIL (AIK,Y,FE,ELEM,NELE,NGAS,NTOT,IND)

AIK - Array of elements in each species Dimension (NELE,NTOT)

Y - Array of initial guesses of moles of each species Dimension (NTOT)

FE - Array of free energies of each species Dimension (NTOT)

ELEM- Array of amount of each element present Dimension (NELE)

NELE- Number of elements

NGAS- Number of gaseous species

NTOT- Total number of species

IND - Error indicator, set to -1 if other than the last solid disappeared, and set to -7 if matrix is singular.

After the CALL EQUIL the user will wish to test IND to determine if an error has occurred.

An Example, $C_4H_8N_8O_8$

$\downarrow i \quad \rightarrow k$

	AIK	C	H	N	O	FREE ENERGY (FE)	NO MOLES (Y)
1.	H_2O	0.	2.	0.	1.	-2.28	4.0
2.	H_2	0.	2.	0.	0.	9.56	0.01
3.	O_2	0.	0.	0.	2.	7.14	0.01
4.	CO_2	1.	0.	0.	2.	-1.25	2.0
5.	CO	1.	0.	0.	1.	4.62	0.01
6.	NH_3	0.	3.	1.	0.	9.79	0.01
7.	H	0.	1.	0.	0.	18.42	0.01
8.	NO	0.	0.	1.	1.	12.10	0.01
9.	N_2	0.	0.	2.	0.	10.25	4.0
10.	OH	0.	1.	0.	1.	13.35	0.01
11.	C_{Solid}	1.	0.	0.	0.	2.99	2.0

AIK(I) for I = 1 to NAIK where NAIK = (NTOT)*(NELE) will be stored in order as a floating point 0., 2., 0., 1., 0., 2., 0., 0., etc.

Y(I) for I = 1 to NTOT will be stored in order as a floating point 4, 0.01, 0.01, 2., etc.

FE(I) for I = 1 to NTOT will be stored in order as a floating point -2.28, 9.56, 7.14, -1.25, etc.

ELEM for I = 1 to NELE will be stored in order as a floating point 4., 8., 8., 8.

NELE is 4, NGAS is 10, NTOT is 11.

The answers will be stored in the same order starting in location Y.

The free energy of each species is of the form

$$F^* = \frac{\mu_i}{RT} - \ln X_i = \left(\frac{F^o - H^o_o}{RT}\right)_i + \left(\frac{\Delta H^o_f}{RT}\right)_i + \ln P$$

+ imperfection terms.

RULES

1. All the gaseous species must be given first, followed by the solid species.
2. If any one solid may not be present, it must be listed last.
3. There must be as many species as elements.
4. Not all the species may be multiples of each other.
5. Initial guesses are best if they satisfy the mass balance constraints; however, any reasonable guesses will probably be satisfactory.

B. FORTRAN Linear Feedback Subroutine. This subroutine solves F(x) = 0 for X by iteration.

The Method (given X guessed, ratio, and max zero).

1. Initial entry
   a. If X guessed = 0., set it to 1.
   b. Set count = 1 and XP = X guessed.
   c. Exit to get F(XP).
2. Second entry
   a. Set XN2 = XP, FN2 = F(XP), FN = F(XP), and count = 2.
   b. If |FN2| < max zero, set count = 0., X guessed = XP, and exit with XP = the solution.
   c. Otherwise, set XP = (X guessed)*(ratio) and exit to get F(XP).
3. Third entry
   a. Set XN1 = XP, FN1 = F(XP), FN = F(XP), and count = 3.
   b. If |FN1| < max zero, set count = 0., X guessed = XP, and exit with XP = the solution.
   c. Otherwise, set XP = XN1 - FN1 $\left(\frac{XN1-XN2}{FN1-FN2}\right)$ and exit to get F(XP).
4. Fourth and succeeding entries
   a. If the count > 1000, exit with count = - count.
   b. Otherwise, set XN = XP, FN = F(XP), and count = count + 1.
   c. If XN = XN1 or FN = FN1, exit with count = - count.
   d. If FN < max zero, set count = 0, X guessed = XP, and exit with XP = the solution.
   e. Otherwise, set XP = XN - FN $\left(\frac{XN-XN1}{FN-FN1}\right)$.
   f. If FN and FN1 are of opposite signs, set XN2 = XN1, FN2 = FN1, XN1 = XN, FN1 = FN, and exit to get F(XP).
   g. If FN and FN2 are of the same sign, set XN2 = XN1, FN2 = FN1, XN1 = XN, FN1 = FN, and exit to get F(XP).
   h. If XP lies between XN and XN2, set XN1 = XN, FN1 = FN, and exit to get F(XP).

i. Otherwise, set $XP = XN - FN \left(\frac{XN-XN2}{FN-FN2}\right)$, $XN1 = XN$, $FN1 = FN$, and exit to get F(XP).

Calling Sequence

CALL LFB (XP,FP,TX)

XP - value of X to calculate F(X)

FP - F(XP)

TX - an array of dimension 10

TX(1) - X guessed

TX(2) - ratio

TX(3) - max zero

TX(4) - XN

TX(5) - FN

TX(6) - XN1

TX(7) - FN1

TX(8) - XN2

TX(9) - FN2

TX(10) - count

On the initial call to LFB, TX(10) must be ≤ 0.

On return from LFB,

TX(10) = 0 if a solution has been found. XP is that solution.

TX(10) > 0. Calculate F(XP) and place in FP.

TX(10) < 0. Error in the calculation (set to negative count) if a) too many iterations (1000), b) two successive XP's are equal, or c) two successive FP's are equal.

C. FORTRAN Thermodynamic Function Subroutine. This subroutine computes the ideal gas thermodynamic functions from a fit of the entropy.

Description

Input is A, B, C, D, E, IC, and the temperature.

$$SO = A + BT + CT^2 + DT^3 + ET^4.$$

$$H - HO = \frac{BT^2}{2} + \frac{2CT^3}{3} + \frac{3DT^4}{4} + \frac{4ET^5}{5} + IC,$$

$$\text{since} \int \frac{dH}{dt} = \int T\frac{dS}{dT}.$$

$$\frac{F\text{-}HO}{T} = -\left(A + \frac{BT}{2} + \frac{CT^2}{3} + \frac{DT^3}{4} + \frac{ET^4}{4}\right) + \frac{IC}{T},$$

$$\text{since } \frac{F\text{-}HO}{T} = \frac{H\text{-}HO}{T} - SO.$$

Programming Instructions

Calling Sequence

CALL TDF (T,A,IND,ANS)

T = Temperature

A = An array of six coefficients A,B,C,D,E,IC

IND = 0 for SO, 1 for H - HO, 2 for F-HO/T

ANS = Result

D. FORTRAN Cowan Solid Equation of State Subroutine.

This subroutine computes the solid volume for a given pressure and temperature, and the thermodynamic imperfection terms for a given pressure, temperature, and volume.

The Formulas

1. To find the volume:

   a. If incompressible, $V_s = V_o$,

   b. Otherwise, linear feedback on ρ_s with $\rho_{guessed} = 1.1[TX(2)]\rho_o$, until error is less than $1.0 \times 10^{-9}[TX(3)]$,

$$T_v = (T)/R_5$$

$$0 = A_s + B_s\rho_s + C_s\rho_s^2 + D_s\rho_s^3 + E_s\rho_s^4$$
$$+ (A1+A2\rho_s)T_v + \left(C1 + \frac{C2}{\rho_s} + \frac{C3}{\rho_s^2}\right)T_v^2 - P.$$

2. To find the imperfection free energy (F_s'):

   a. If incompressible, $F_s' = (P)(V_o)(MOLWT)$,

   b.

$$F_s' = (MOLWT)\Big\{PV_s - \Big[\left(A_sV_s + B_s\ln V_s - \frac{C_s}{V_s} - \frac{D_s}{2V_s^2} - \frac{E_s}{3V_s^3}\right)$$
$$+ \left(A1V_s + A2\ln V_s\right)T_v + \left(C1V + \frac{C_2V_s^2}{2} + \frac{C_3V^3}{3}\right)T_v^2\Big]_{V_o}^{V}\Big\}.$$

Units are Mbar-cc/mole.

3. To find imperfection enthalpy (E'_s):

   a. If incompressible, $E_s' = 0$,

   b. $$E'_s = (MOLWT)\Big[\left(C1V_s + \frac{C2V_s^2}{2} + \frac{C3V_s^3}{3}\right)T_v^2$$
$$- \left(A_sV_s + B_s\ln V_s - \frac{C_s}{V_s} - \frac{D_s}{2V_s^2} - \frac{E_s}{3V_s^3}\right)\Big]_{V_o}^{V}.$$

Units are Mbar-cc/mole.

4. To find the imperfection entropy (S_s'):

   a. If incompressible, $S_s' = 0$,

   b. $$S'_s = (MOLWT)\Big[(A1V_s + A2\ln V_s) + 2T_v$$
$$\left(CIV_s + \frac{C2V_s^2}{2} + \frac{C3V_s^3}{3}\right)\Big]_{V_o}^{V}.$$

Units are Mbar-cc/v-mole.

Programming Instructions

Calling Sequence

CALL SES (P,A,IND,ANS).

P = An array of 3 P(1) Pressure (Mbar),
P(2) temperature (^oK),
P(3) volume (cc/g for imperfection terms).

A = An array of 12 equation of state coefficients VO, A_s, B_s, C_s, D_s, E_s, A1, A2, C1, C2, C3, MOLWT.

IND = 0 for volume, 1 for free energy, 2 for energy, 3 for entropy and set equal to -1 for error in linear feedback on volume.

ANS = Answer. If IND is 0 the answer is also put in P(3).

E. FORTRAN Minimum of a Parabola Subroutine. This subroutine computes the minimum of a function D = f(P) by approximating it with a parabola.

The formula for min P from 3 sets of D and P is

$$P_{min} = (\tfrac{1}{2})\frac{P_1^2(D_3-D_2) + P_2^2(D_1-D_3) + P_3^2(D_2-D_1)}{P_1(D_3-D_2) + P_2(D_1-D_3) + P_3(D_2-D_1)}$$

Programming Instructions

Calling Sequence

CALL MIND (P,D,PG).

P = Calculated P (Pmin).

D = Calculated D (calculated by users code).

PG = An array of 4 PG(1) P guessed,
PG(2) Ratio of next two guesses
PG(3) Definition of when minimum is reached,
PG(4) Cycle count - set to zero on solution, set to -1 if more than 1000 iterations.

APPENDIX II
FORTRAN LISTING OF THE CODE

The order of the code is input; output; dependent subroutines 1, 2, 2A, 3, 4, 4A, 5; and independent subroutines EQUIL, LFB, MIND, SES, TDF, LSS, and PFTS.

```
                      PROGRAM BKW (INPUT,OUTPUT,FILM,TAPE12=FILM)
000003                COMMON  X(25),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
                     1FREENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
                     2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,EO,IOEQ,ICJC,IHUG,IPVC,
                     3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
                     4ETOT,VTOT,VPG,FS(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
                     5,VCJ,UCJ,CJT,CJS
000003                COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
                     1,R3,R5,R6,SCALF,PO,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
                     2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)
                     3,ASBOS(10),ASBOSH(10),ASP(100),ASV(100),AST(100),ASE(100),ASG(100)
                     4,ASUP(100),VAHX(2500),ALGV(100),CPRIME,DECIP,AMINP,AINCP,AMAXP
                     5,ALX(101),FITP(100),FITT(100),FITE(100),PCOEF(5),TCOEF(5),ECOEF(5)
                     6,W(100),DELY(100),SB(5),T(5),A(5,5),ALGP(100),DPDV(100),IT,IW
                     7,ALGF(100),VBOS2,HUGB2,NSF,NAIK,VO
000003                COMMON /NAMES/ NAM(25),NAMS(5),NAME(10),LABEL(12)
000003                COMMON/SUBVAR/AMAXE,AMINX,AMINY,TX(10)
000003                DIMENSION  ATHRHO(4),NOVAR(25),VAR(25)
              C       THE READING OF INPUT DATA
000003              1 READ 901,IOEQ,ICJC,IHUG,IPVC,IGRP,IDIC,IRHO,IONL,IMIS,IEXT
000033                READ 904, LABEL
000041                READ 901,M,N,NT
000053                IF(M.GT.10) GO TO 410
000057                IF(NT.GT.25) GO TO 410
000062                READ 902,ALPHA,BETA,THETA,AKAPPA
000075                READ 905,(NAME(I),I=1,M)
000110                READ 902,(ELEM(I),I=1,M)
000123                READ 902,RHO,AMOLWT,EO
000135                READ 902, TEMP,PRESS
```

```
000145           READ 905,(NAM(I),I=1,NT)
000160           READ 902,(X(I),I=1,NT)
000173           NTDF=(8)*NT
000176           READ 902,(THERC(I),I=1,NTDF)
000210           IF(N.EQ.NT) GO TO 3
000212           NSF = (NT-N)
000213           IF(NSF.GT.5) GO TO 410
000216           READ 905,(NAMS(I),I=1,NSF)
000230           DO 7 I=1,NSF
000232           READ 902,(SOLEQS(J,I),J=1,12)
000245       7   CONTINUE
000250       3   NAIK=(NT)*(M)
000253           READ 902,(AIK(I)    ,I=1,NAIK)
000265      10   IF(IRHO.LT.1) GO TO 11
000267           IF(IRHO.GT.4) GO TO 200
000272           READ 902,(ATHRHO(I),I=1,IRHO)
        C        EXTRA INPUT FEATURE
000304      11   IF(IEXT.LT.1)GO TO 200
000306           IF(IEXT.GT.25) GO TO 200
000311           DO 12 I=1,IEXT
000312           READ 906, (NOVAR(I),VAR(I))
000321      12   CONTINUE
000324     299   DO 380 I=1,IEXT
000326           IF(NOVAR(I)-1)  300,301,302
000331     301   VBOS(1)=VAR(I)
000333     302   IF(NOVAR(I) -2) 300,303,304
000337     303   VBOS(2)=VAR(I)
000341     304   IF(NOVAR(I)-3) 300,305,306
000345     305   VBOS(3)=VAR(I)
000347     306   IF(NOVAR(I)-4) 300,307,308
000353     307   EXITME=VAR(I)
000355     308   IF(NOVAR(I)-5) 300,309,310
000361     309   HUGBOS(1)=VAR(I)
000363     310   IF(NOVAR(I)-6) 300,311,312
000367     311   HUGBOS(2)=VAR(I)
000371     312   IF(NOVAR(I)-7) 300,313,314
000375     313   HUGBOS(3)=VAR(I)
000377     314   IF(NOVAR(I)-8) 300,315,316
000403     315   PO=VAR(I)
000405     316   IF(NOVAR(I)-9) 300,317,318
000411     317   CJBOS(2)=VAR(I)
000413     318   IF(NOVAR(I)-10) 300,319,320
000417     319   CJBOS(3)=VAR(I)
000421     320   IF(NOVAR(I)-11) 300,321,322
000425     321   APGCJ=VAR(I)
000427     322   IF(NOVAR(I)-12) 300,323,324
000433     323   BPGCJ=VAR(I)
000435     324   IF(NOVAR(I)-13)300,325,326
000441    325    AMHUGP=VAR(I)
000443     326   IF(NOVAR(I)-14)300,327,328
000447     327   DELP=VAR(I)
000451     328   IF(NOVAR(I)-15)300,329,330
000455     329   CPRIME=VAR(I)
000457     330   IF(NOVAR(I)-16)300,331,332
000463     331   DECIP=VAR(I)
000465     332   IF(NOVAR(I)-17)300,333,334
000471     333   AMINP=VAR(I)
000473     334   IF(NOVAR(I)-18)300,335,336
000477     335   AINCP=VAR(I)
000501     336   IF(NOVAR(I)-19)300,337,338
000505     337   AMAXP=VAR(I)
000507     338   IF(NOVAR(I)-20)300,339,340
000513     339   ASBOS(2)=VAR(I)
000515     340   IF(NOVAR(I)-21)300,341,342
000521     341   ASBOS(3)=VAR(I)
000523     342   IF(NOVAR(I)-22) 300,343,344
000527     343   ASBOSH(2)=VAR(I)
000531     344   IF(NOVAR(I)-23) 300,345,346
000535     345   ASBOSH(3)=VAR(I)
000537     346   IF(NOVAR(I)-24) 300,347,348
```

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000543      347 VBOS2=VAR(I)
000545      348 IF(NOVAR(I)-25) 300,349,350
000551      349 HUGB2=VAR(I)
000553      350 IF(NOVAR(I)-26) 300,351,352
000557      351 AMAXE = VAR(I)
000561      352 IF(NOVAR(I)-27) 300,353,354
000565      353 AMINX = VAR(I)
000567      354 IF(NOVAR(I)-28) 300,355,356
000573      355 AMINY = VAR(I)
000575      356 IF(NOVAR(I)-29) 300,357,358
000601      357 TX(2) = VAR(I)
000603      358 IF(NOVAR(I)-30) 300,359,300
000606      359 TX(3) = VAR(I)
000610     300  PRINT 992, NOVAR(I),VAR(I)
000620          WRITE (12,992) NOVAR(I),VAR(I)
000630      380 CONTINUE
          C     MAIN CONTROL
000633      200 IF(IHUG.GT.0) ICJC=1
000636          IF(IPVC.GT.0) ICJC=1
000641          VO=1./RHO
000643          IF(IOEQ.EQ.0) GO TO 201
000644          CALL SYS1 (IND)
000646          IF(IND.LT.0) GO TO 400
000647          CALL CJPNT
000650      201 IF(ICJC.EQ.0) GO TO 202
000651          CALL SYS3(IND)
000653          IF(IND.LT.0) GO TO 400
000654          CALL CJPNT
000655      202 IF(IHUG.EQ.0) GO TO 203
000656          CALL SYS5 (IND)
000660          IF(IND.LT.0) GO TO 400
000661          CALL HUGPNT
000662      203 IF(IPVC.EQ.0) GO TO 204
000663          CALL SYS4A (IND)
000665          IF(IND.LT.0) GO TO 400
000666          CALL ISPNT
000667      204 IF(IRHO.EQ.0) GO TO 205
000670          RHO=ATHRHO(IRHO)
000672          IRHO=IRHO-1
000673          HUGBOS=HUGB2
000675          VBOS=VBOS2
000676          GO TO 200
000677      205 VBOS=VBOS2
000701          HUGBOS=HUGB2
000702          GO TO 1
          C     ERROR RETURN
000703      400 IF(IND.EQ.-1) GO TO 401
000705          IF(IND.EQ.-2) GO TO 402
000707          IF(IND.EQ.-3) GO TO 403
000711          IF(IND.EQ.-4) GO TO 404
000713          IF(IND.EQ.-5) GO TO 405
000715          IF(IND.EQ.-6) GO TO 406
000717          IF(IND.EQ.-7) GO TO 407
000721      401 PRINT 990
000725          PRINT 981
000731          PRINT 990
000735          CALL CJPNT
000736          STOP
000740      402 PRINT 990
000744          PRINT 982
000750          PRINT 990
000754          CALL CJPNT
000755          STOP
000757      403 PRINT 990
000763          PRINT 983
000767          PRINT 990
000773          CALL CJPNT
000774          STOP
000776      404 PRINT 990
001002          PRINT 984
```

```
001006         PRINT 990
001012         CALL CJPNT
001013         CALL HUGPNT
001014         STOP
001016     405 PRINT 990
001022         PRINT 985
001026         PRINT 990
001032         CALL CJPNT
001033         STOP
001035     406 PRINT 990
001041         PRINT 986
001045         PRINT 990
001051         CALL CJPNT
001052         CALL ISPNT
001053         STOP
001055     407 PRINT 990
001061         PRINT 987
001065         PRINT 990
001071         CALL CJPNT
001072         STOP
001074     410 PRINT 990
001100         PRINT 991
001104         PRINT 990
001110         CALL CJPNT
001111         STOP
001113    901  FORMAT (12I5)
001113     902 FORMAT (4E18.11)
001113     904 FORMAT (12A6)
001113    905  FORMAT (11A6)
001113    906  FORMAT(1I5,1E18.11)
         C     ERROR RETURN FORMATS
001113     990 FORMAT (101H1********ERROR***********ERROR****************ERROR****
              1*******ERROR**********ERROR********ERROR******)
001113     981 FORMAT (54H AN ERROR IN LFB INTERATING ON  GAS VOLUME  SYS1       )
001113     982 FORMAT (54H AN ERROR IN LFB INTERATING ON  SOLID VOLUME  SYS1     )
001113     983 FORMAT (54H AN ERROR IN EQUIL OTHER THAN LAST SOLID DISAPPEARED  )
001113     984 FORMAT (54H AN ERROR IN LFB INTERATING ON HUGONIOT TEMP  SYS2A   )
001113     985 FORMAT (54H AN ERROR IN MIND,USED BY SYS3,MORE THAN 1000 INTERATE)
001113     986 FORMAT (54H AN ERROR IN LFB ITERATING ON P FOR ISENTROPE    SYS4A)
001113     987 FORMAT (54H AN ERROR IN EQUIL  SINGULAR MATRIX  FROM LSS  SYS1   )
001113    991  FORMAT(109H THE INPUT DIMENSIONS ARE TOO LARGE ***CAN ONLY HAVE 10
              1 ELEMENTS, 25 SPECIES OF WHICH ONLY 5 MAY BE SOLIDS   )
001113    992  FORMAT (27H1 CONSTANT WITH IDENITY NO ,1I5, 4H IS ,1PE18.11)
001113         END
```

```
               SUBROUTINE CJPNT
         C     THE PRINTING OF THE C J RESULTS
000002         COMMON  X(25),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
              1FREENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
              2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,EO,IOEQ,ICJC,IHUG,IPVC,
              3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
              4ETOT,VTOT,VPG,ES(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
              5,VCJ,UCJ,CJT,CJS
000002         COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
              1,R3,R5,R6,SCALF,PO,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
              2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)
              3,ASBOS(10),ASBOSH(10),ASP(100),ASV(100),AST(100),ASE(100),ASG(100)
              4,ASUP(100),VAHX(2500),ALGV(100),CPRIME,DECIP,AMINP,AINCP,AMAXP
              5,ALX(101),FITP(100),FITT(100),FITE(100),PCOEF(5),TCOEF(5),ECOEF(5)
              6,W(100),DELY(100),SB(5),T(5),A(5,5),ALGP(100),DPDV(100),IT,IW
              7,ALGF(100),VBOS2,HUGB2,NSF,NAIK,VO
000002         COMMON /NAMES/ NAM(25),NAMS(5),NAME(10),LABEL(12)
000002         PRINT 902
000006         PRINT 900,LABEL
000014         PRINT 903, M
000022         PRINT 904, N
```

```
000030          PRINT 905, NSF
000036          PRINT 906
000042          PRINT 907,ALPHA,BETA,THETA,AKAPPA
000056          PRINT 908
000062          DO 10 I=1,M
000064          PRINT 909, ELEM(I), NAME(I)
000075       10 CONTINUE
000100          PRINT 910, RHO
000105          PRINT 911, AMOLWT
000113          PRINT 912, EO
000121          PRINT 913
000125          DO 11 I=1,NSF
000127          PRINT 914, NAMS(I),(SOLEQS(J,I),J=1,6)
000145          PRINT 915,(SOLEQS(J,I),J=7,12)
000161       11 CONTINUE
000164          PRINT 916
000167          PRINT 917,(AIK(I),I=1,NAIK)
000202          PRINT 902
000206          PRINT 900,LABEL
000214          PRINT 918,PCJ
000222          PRINT 919,DETVEL
000230          PRINT 920,CJT
000236          PRINT 929,VCJ
000244          PRINT 921,GAMMA
000252          PRINT 922,VGAS,XBAR
000262          PRINT 923
000266          DO 12 I=1,NSF
000270          PRINT 924,NAMS(I),VSOL(I)
000301       12 CONTINUE
000304          PRINT 925
000307          PRINT 926
000313          DO 13 I=1,NT
000315          PRINT 927,NAM(I),X(I),(THERC(J,I),J=1,5)
000336          PRINT 928,(THERC(J,I),J=6,8)
000352       13 CONTINUE
000355          IF (IGRP.EQ.0) RETURN
000356          WRITE (12,902)
000362          WRITE (12,900) LABEL
000370          WRITE (12,903) M
000376          WRITE (12,904) N
000404          WRITE (12,905) NSF
000412          WRITE (12,906)
000416          WRITE (12,907) ALPHA,BETA,THETA,AKAPPA
000432          WRITE (12,908)
000436          DO 20 I=1,M
000440          WRITE (12,909) ELEM(I),NAME(I)
000451       20 CONTINUE
000454          WRITE (12,910) RHO
000461          WRITE (12,911) AMOLWT
000467          WRITE (12,912) EO
000475          WRITE (12,913)
000501          DO 21 I=1,NSF
000503          WRITE (12,914) NAMS(I),(SOLEQS(J,I),J=1,6)
000521          WRITE (12,915)(SOLEQS(J,I),J=7,12)
000535       21 CONTINUE
000540          WRITE (12,916)
000543          WRITE (12,917)(AIK(I),I=1,NAIK)
000556          WRITE (12,902)
000562          WRITE (12,900) LABEL
000570          WRITE (12,918) PCJ
000576          WRITE (12,919) DETVEL
000604          WRITE (12,920) CJT
000612          WRITE (12,929) VCJ
000620          WRITE (12,921) GAMMA
000626          WRITE (12,922)VGAS,XBAR
000636          WRITE (12,923)
000642          DO 22 I=1,NSF
000644          WRITE (12,924) NAMS(I),VSOL(I)
000655       22 CONTINUE
000660          WRITE (12,925)
```

```
000663         WRITE (12,926)
000667         DO 23  I=1,NT
000671         WRITE (12,927) NAM(I),X(I),(THERC(J,I),J=1,5)
000712         WRITE (12,928) (THERC(J,I),J=6,8)
000726      23 CONTINUE
000731         RETURN
000731     900 FORMAT(12A6)
000731     901 FORMAT(11A6)
000731     902 FORMAT (46H1 A FORTRAN BKW CALCULATION FOR THE EXPLOSIVE )
000731     903 FORMAT (//,28H THE NUMBER OF ELEMENTS IS  ,I5)
000731     904 FORMAT (//,30H THE NUMBER OF GAS SPECIES IS ,I5)
000731     905 FORMAT (//,32H THE NUMBER OF SOLID SPECIES IS ,I5)
000731     906 FORMAT (//,41H THE BKW EQUATION OF STATE PARAMETERS ARE)
000731     907 FORMAT ( 8H  ALPHA=,1PE18.11,6H BETA=,1PE18.11,7H THETA=,1PE18.11,
              17H KAPPA=,1PE18.11)
000731     908 FORMAT (//,40H THE COMPOSITION OF THE EXPLOSIVE IS     )
000731     909 FORMAT (5H     ,1PE18.11,10H MOLES OF ,1A6)
000731     910 FORMAT (//,33H THE DENSITY OF THE EXPLOSIVE IS ,1PE18.11,10H, GRAM
              1S/CC )
000731     911 FORMAT (//,25H THE MOLECULAR WEIGHT IS ,1PE18.11, 6H GRAMS)
000731     912 FORMAT(//,37H THE HEAT OF FORMATION AT 0 DEG K IS ,1PE18.11,29H CA
              1LORIES PER FORMULA WEIGHT )
000731     913 FORMAT (//,109H THE SOLID (COWAN) EQUATION OF STATE PARAMETERS
              1VO, AS, BS, CS, DS, ES,     A1, A2, C1, C2, C3, ATOMIC WT )
000731     914 FORMAT (//,1A6,6(2X,1PE18.11))
000731     915 FORMAT (6H      ,6(2X,1PE18.11))
000731     916 FORMAT (//,59H THE INPUT DETONATION PRODUCT ELEMENTAL COMPOSITION
              1MATRIX )
000731     917 FORMAT (12(3X,1PF7.1))
000731     918 FORMAT (//,32H THE COMPUTED CJ PRESSURE IS     ,1PE18.11,13H    MEG
              1ABARS )
000731     919 FORMAT (//,40H THE COMPUTED DETONATION VELOCITY IS     ,1PE18.11,19
              1H    CM/MICROSECOND )
000731     920 FORMAT(//,35H THE COMPUTED CJ TEMPERATURE IS     ,1PE18.11,19H    D
              1EGREES KELVIN )
000731     921 FORMAT (//,23H THE COMPUTED GAMMA IS ,1PE18.11)
000731     922 FORMAT (//,28H THE VOLUME OF THE GAS IS    ,1PE18.11,35H   CC/MOLE
              1OF GAS AND THERE ARE     ,1PE18.11,15H   MOLES OF GAS)
000731     923 FORMAT (//,25H SOLID    VOLUME IN CC/GM)
000731     924 FORMAT (1A6,3X,1PE18.11)
000731     925 FORMAT(//,116H THE C-J COMPOSITION OF THE DETONATION PRODUCTS AND
              1THE INPUT COEFFICIENTS TO THE THERMODYNAMIC FITS FOR EACH SPECIE)
000731     926 FORMAT (//,116H SPECIE    NO OF MOLES         COEFFICIENTS A,B,C,D,E,
              1 THE INTEGRATION CONSTANT, HEAT OF FORMATION IN CAL/MOLE,COVOLUME)
000731     927 FORMAT (1A6,3X,1PE18.11,5(2X,1PE18.11))
000731     928 FORMAT (27H                                 ,3(2X,1PE18.11))
000731     929 FORMAT (//,26H THE COMPUTED CJ VOLUME    ,1PE18.11,21H  CC/GM OF EX
              1PLOSIVE )
000731         END
```

```
               SUBROUTINE HUGPNT
          C    THE PRINTING AND GRAPHING OF HUGONIOT RESULTS
000002         COMMON  X(25),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
              1FREENE(25),XN1(25),FSOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
              2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,EO,IOEQ,ICJC,IHUG,IPVC,
              3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
              4ETOT,VTOT,VPG,FS(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
              5,VCJ,UCJ,CJT,CJS
000002         COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
              1,R3,R5,R6,SCALF,PO,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
              2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)
              3,ASBOS(10),ASBOSH(10),ASP(100),ASV(100),AST(100),ASE(100),ASG(100)
              4,ASUP(100),VAHX(2500),ALGV(100),CPRIME,DECIP,AMINP,AINCP,AMAXP
              5,ALX(101),FITP(100),FITT(100),FITE(100),PCOEF(5),TCOEF(5),ECOEF(5)
              6,W(100),DELY(100),SB(5),T(5),A(5,5),ALGP(100),DPDV(100),IT,IW
```

```
                 7,ALGF(100),VBOS2,HUGB2,NSF,NAIK,VO
000002            COMMON /NAMES/ NAM(25),NAMS(5),NAME(10),LABEL(12)
000002            DATA ICHAR/055/
000002            PRINT 902
000006            PRINT 900,LABEL
000014            K=1
000015            DO 10 I=1,IT
000017            PRINT 903,HUGP(I),HUGV(I),HUGT(I)
000033            IF ( I.GT.IW) GO TO 12
000037            PRINT 904,HUGUS(I),HUGUP(I)
000050        12  PRINT 905
000054            DO 11 J=1,NT
000056            PRINT 906,NAM(J),VAHX(K)
000067            K=K+1
000071         11 CONTINUE
000073         10 CONTINUE
000076            IF (IGRP.EQ.0) RFTURN
000077            WRITE (12,902)
000103            WRITE (12,900) LABEL
000111            K=1
000112            DO 20 I=1,IT
000114            WRITE (12,903) HUGP(I),HUGV(I),HUGT(I)
000130            IF ( I.GT.IW) GO TO 22
000134            WRITE (12,904) HUGUS(I),HUGUP(I)
000145        22  WRITE (12,905)
000151            DO 21 J=1,NT
000153            WRITE (12,906) NAM(J),VAHX(K)
000164            K=K+1
000166         21 CONTINUE
000170         20 CONTINUE
            C     GRAPH PRFSSURE VS  VOLUME
000173            CALL ADV(1)
000174            CALL DGA (123,1023,0,900,0.,1.0,1.,0.)
000204            CALL DLNLN (10,10)
000206            CALL SLLIN (10,2)
000210            CALL SBLIN (10,2)
000212            CALL PLOT (IT,HUGV,1,HUGP,1,ICHAR,1)
000221            CALL LINCNT (60)
000223            WRITE (12,900) LABEL
000231            WRITE (12,907)
            C     GRAPH PRESSURE  VS PARTICLE VELOCITY
000235            CALL ADV(1)
000237            CALL DGA (123,1023,0,900,0.,1.0,1.0,0.)
000247            CALL DLNLN (10,10)
000251            CALL SLLIN (10,2)
000253            CALL SBLIN (10,2)
000255            CALL PLOT (IW,HUGUP,1,HUGP,1,ICHAR,1)
000264            CALL LINCNT (60)
000266            WRITE (12,900) LABEL
000274            WRITE (12,908)
            C     GRAPH SHOCK VELOCITY VS PARTICLE VELOCITY
000300            CALL ADV(1)
000302            CALL DGA (123,1023,0,900,0.,1.,1.5,0.5)
000312            CALL DLNLN(10,10)
000314            CALL SLLIN (10,2)
000316            CALL SBLIN (10,2)
000320            CALL PLOT (IW,HUGUP,1,HUGUS,1,ICHAR,1)
000327            CALL LINCNT (60)
000331            WRITE (12,900) LABEL
000337            WRITE (12,909)
000343            RETURN
000344        900 FORMAT(12A6)
000344        902 FORMAT (50H1 THE BKW HUGONIOT FOR THE DETONATION PRODUCTS OF )
000344        903 FORMAT (//,12H PRESSURE = ,1PE18.11,10H VOLUME = ,1PE18.11,15H TEM
                 1PERATURE = ,1PE18.11)
000344        904 FORMAT (18H SHOCK VELOCITY = ,1PE18.11,20H PARTICLE VELOCITY =,1PE
                 118.11,50H UNITS ARE MBARS,CC/GM, DEG K, AND CM/MICROSECOND )
000344        905 FORMAT (//,22H  SPECIE   NO OF MOLES)
000344        906 FORMAT (1A6,3X,1PE18.11)
000344        907 FORMAT (//,46H   PRESSURE (MBARS) - VOLUME (CC/GM) HUGONIOT )
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000344      908 FORMAT (//,61H   PRESSURE (MBARS) - PARTICLE VELOCITY (CM/USEC)
               1HUGONIOT )
000344      909 FORMAT (//,50H   SHOCK VELOCITY - PARTICLE VELOCITY HUGONIOT     )
000344          END




                SUBROUTINE ISPNT
          C     THE PRINTING AND GRAPHING OF ISENTROPE RESULTS
000002          COMMON  X(25),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
               1FREENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
               2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,EO,IOEQ,ICJC,IHUG,IPVC,
               3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
               4ETOT,VTOT,VPG,ES(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
               5,VCJ,UCJ,CJT,CJS
000002          COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
               1,R3,R5,R6,SCALF,PO,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
               2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)
               3,ASBOS(10),ASBOSH(10),ASP(100),ASV(100),AST(100),ASE(100),ASG(100)
               4,ASUP(100),VAHX(2500),ALGV(100),CPRIME,DECIP,AMINP,AINCP,AMAXP
               5,ALX(101),FITP(100),FITT(100),FITE(100),PCOEF(5),TCOEF(5),ECOEF(5)
               6,W(100),DELY(100),SB(5),T(5),A(5,5),ALGP(100),DPDV(100),IT,IW
               7,ALGF(100),VBOS2,HUGB2,NSF,NAIK,VO
000002          COMMON /NAMES/ NAM(25),NAMS(5),NAME(10),LABEL(12)
000002          DATA ICHAR /044/
000002          DATA ICHAR2 /063/
000002          PRINT 902
000006          PRINT 900,LABEL
000014          PRINT 903,(PCOEF(I),I=1,5)
000026          PRINT 904,(TCOEF(I),I=1,5)
000040          PRINT 905,(ECOEF(I),I=1,5)
000052          PRINT 906,CPRIME
000060          PRINT 907
000064          DO 10  I=1,IT
000066          PRINT 908,ASP(I),ASV(I),AST(I),ASE(I),ASG(I),ASUP(I)
000113       10 CONTINUE
000116          PRINT 909
000121          PRINT 910
000125          DO 11 I=1,IT
000127          PRINT 908,ASP(I),FITP(I),AST(I),FITT(I),ASE(I),FITE(I)
000154       11 CONTINUE
000157          PRINT 911
000162          PRINT 912,(NAM(I),I=1,NT)
000175          K = 1
000176          L = NT
000200          DO 12 I=1,IT
000201          PRINT 908,ASP(I),(VAHX(J),J=K,L)
000216          K = K + NT
000220          L = L + NT
000221       12 CONTINUE
000223          IF(IGRP.EQ.0) RETURN
000225          WRITE (12,902)
000231          WRITE (12,900) LABEL
000237          WRITE (12,903) (PCOEF(I),I=1,5)
000251          WRITE (12,904) (TCOEF(I),I=1,5)
000263          WRITE (12,905) (ECOEF(I),I=1,5)
000275          WRITE (12,906) CPRIME
000303          WRITE (12,907)
000307          DO 20 I=1,IT
000311          WRITE (12,908)ASP(I),ASV(I),AST(I),ASE(I),ASG(I),ASUP(I)
000336       20 CONTINUE
000341          WRITE(12,909)
000344          WRITE (12,910)
000350          DO 21 I=1,IT
000352          WRITE (12,908)ASP(I),FITP(I),AST(I),FITT(I),ASE(I),FITE(I)
000377       21 CONTINUE
000402          WRITE (12,911)
000405          WRITE (12,912) (NAM(I),I=1,NT)
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000420          K = 1
000421          L = NT
000423          DO 22 I=1,IT
000424          WRITE (12,908) ASP(I),(VAHX(J),J=K,L)
000441          K = K + NT
000443          L = L + NT
000444       22 CONTINUE
        C       GRAPH LOG SET UPS
000446          DO 30 I = 1,IT
000450          ASP(I)=ALOG10(ASP(I))
000455          ASV(I)=ALOG10(ASV(I))
000462       30 CONTINUE
000465          APCJ = ALOG10(PCJ)
000467          AVCJ=ALOG10(VCJ)
        C       GRAPH LOG PRESSURE VS VOLUME
000471          CALL ADV (1)
000472          CALL DGA (123,1023,0,900,-1.,+2.,+0.,-4.)
000502          CALL DLGLG
000503          CALL SLLOG
000504          CALL SBLOG
000505          CALL PLOT(IT,ASV ,1,ASP,1,ICHAR,0)
000514          CALL PLOT(1,AVCJ,1,APCJ,1,ICHAR2,0)
000523          CALL LINCNT (60)
000525          WRITE (12,900) LABEL
000533          WRITE (12,913)
        C       GRAPH TEMPERATURF VS LOG VOLUME
000537          CALL ADV(1)
000541          CALL DGA (123,1023,0,900,-1.,+2.,+1.E+4,0.)
000551          CALL DLGLN(10)
000553          CALL SLLIN(10,1)
000555          CALL SBLOG
000556          CALL PLOT(IT,ASV,1,AST,1,ICHAR,0)
000565          CALL PLOT(1,AVCJ,1,CJT,1,ICHAR2,0)
000574          CALL LINCNT (60)
000576          WRITE (12,900)LABEL
000604          WRITE (12,914)
        C       GRAPH PRESSURE VS PARTICLE VELOCITY
000610          CALL ADV(1)
000612          CALL DGA(123,1023,0,900,0.,+1.,+0.,-4.)
000622          CALL DLNLG(10)
000624          CALL SLLOG
000625          CALL SBLIN(10,2)
000627          CALL PLOT (IW,ASUP,1,ASP,1,ICHAR,1)
000636          CALL PLOT (1,UCJ,1,APCJ,1,ICHAR2,0)
000645          CALL LINCNT (60)
000647          WRITE (12,900)LABEL
000655          WRITE (12,915)
000661          RETURN
000662      900 FORMAT(12A6)
000662      902 FORMAT(44H1 A BKW ISENTROPE THRU BKW CJ PRESSURE FOR  )
000662      903 FORMAT(//,8H LN(P)= ,1PE18.11,3X,1PE18.11,5HLNV   ,1PE18.11,6HLNV*2
               1 ,1PE18.11,6HLNV*3 ,1PE18.11,5HLNV*4)
000662      904 FORMAT(//,8H LN(T)= ,1PE18.11,3X,1PE18.11,5HLNV   ,1PE18.11,6HLNV*2
               1 ,1PE18.11,6HLNV*3 ,1PE18.11,5HLNV*4)
000662      905 FORMAT(//,8H LN(E)= ,1PE18.11,3X,1PE18.11,5HLNP   ,1PE18.11,6HLNP*2
               1 ,1PE18.11,6HLNP*3 ,1PE18.11,5HLNP*4)
000662      906 FORMAT(//,36H THF CONSTANT ADDED TO ENERGIES WAS ,1PE18.11)
000662      907 FORMAT(//,126H    PRESSURE (MBARS)      VOLUME (CC/GM)         TEMPER
               1ATURE (DEG K)  ENERGY+C (MB-CC/GM)  GAMMA (-DLNP/DLNV)    PARTICLE
               2VELOCITY)
000662      908 FORMAT(6(3X,1PE18.11))
000662      909 FORMAT(70H1 THE ISENTROPE STATE VARIABLES AS COMPUTED FROM THE LEA
               1ST SQUARES FIT)
000662      910 FORMAT(//,119H    BKW PRESSURE            FIT PRESSURE             BKW TE
               1MPERATURE          FIT TEMPERATURE      BKW ENERGY + C          FIT ENERG
               2Y)
000662      911 FORMAT (64H1  THE ISENTROPE PRESSURE AND COMPOSITION OF DETONATION
               1 PRODUCTS)
000662      912 FORMAT (20A6)
000662      913 FORMAT (47H  PRESSURE-VOLUME ISENTROPE THRU THE C-J VALUE )
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000662      914 FORMAT (50H  TEMPERATURE -VOLUME ISENTROPE THRU THE C-J VALUE)
000662      915 FORMAT (43H  PRESSURE -PARTICLE VELOCITY ISENTROPE    )
000662          END
```

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                SUBROUTINE  SYS1 (IND)
          C     SYSTEM  I
          C     GIVEN P,T  COMPUTE V
          C     IND IS -1 FOR VGAS LFB ERROR, -2-VSOL LFB ERROR,-3 EQUIL ERROR
000003          COMMON  X(25),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
               1FREENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
               2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,EO,IOEQ,ICJC,IHUG,IPVC,
               3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
               4ETOT,VTOT,VPG,ES(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
               5,VCJ,UCJ,CJT,CJS
000003          COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
               1,R3,R5,R6,SCALF,PO,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
               2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)
               3,ASBOS(10),ASBOSH(10),ASP(100),ASV(100),AST(100),ASE(100),ASG(100)
               4,ASUP(100),VAHX(2500),ALGV(100),CPRIME,DECIP,AMINP,AINCP,AMAXP
               5,ALX(101),FITP(100),FITT(100),FITE(100),PCOEF(5),TCOEF(5),ECOEF(5)
               6,W(100),DELY(100),SB(5),T(5),A(5,5),ALGP(100),DPDV(100),IT,IW
               7,ALGF(100),VBOS2,HUGB2,NSF,NAIK,VO
000003          DATA VBOS2 /+1.5E+1/
000003          DATA VBOS(1)/+1.5E+1/
000003          DATA VBOS(2)/+1.1/
000003          DATA VBOS(3)/+1.E-8/
000003          DATA VBOS(10)/0./
000003          DATA R1/1.98718/
000003          DATA R2/8.31439E-5/
000003          DATA R3/+2.39004905E+4/
000003          DATA ABTOA/0.98692E+6/
000003          DATA  R5/+1.16056E+4/
000003          DATA  R6/+0.4342944819/
000003          DATA EXITME/+2.0E-5/
000003      100 XBAR=0.
000004          DO 101 I=1,N
000006          XBAR=XBAR+X(I)
000011      101 CONTINUE
000013          Z=0.
000014          DO 102 I=1,N
000015          Z=Z+(X(I) /XBAR)*THERC(8,I)
000025      102 CONTINUE
000030          TTA= (TEMP+THETA)**ALPHA
000034          Z=AKAPPA*Z
000036     109  CALL LFB (VGAS,F,VBOS)
000042          IF(VBOS(10)) 103,104,105
000044      103 IND=-1
000045          RETURN
000046      105 W=Z/(VGAS*TTA)
000051          FX=(1.+W*EXP(BETA*W))
000060          F=  FX -(PRESS *VGAS)/(R2*TEMP)
000065          GO TO 109
          C     FIND FREE ENERGIES
000065      104 FGP=-(EXP(BETA*W)-1.)/BETA +(ALOG(FX))
000100          ALNP=ALOG(PRESS*ABTOA)
000105          R1T=(R1)*(TEMP)
000107          R2T=(R2)*(TEMP)
000110          DO 106 J=1,N
000112          CALL TDF (TEMP,THERC(1,J),2,FREENE(J))
000121          FREENE(J)=FREENE(J)/R1+(THERC(7,J)/R1T)+ALNP
               1-(FGP-(AKAPPA)*(THERC(8,J))*(FX-1.)/Z)
000144      106 CONTINUE
000147          IF(N.EQ.NT) GO TO 111
000151          NS=N+1
000153          I = 1
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000154          DO 107 J=NS,NT
000156          CALL TDF(TEMP,THERC(1,J),2,FREENE(J))
000165          FREENE(J)=(FREENE(J))/(R1)+(THERC(7,J)/R1T)
000174          SESP(1)=PRESS
000176          SESP(2)=TEMP
000177          IND=0
000200          SESP(3)=0.
000200          CALL SES(SESP,SOLEQS(1,I),IND,VSOL(I))
000210          IF (IND.EQ.-1) GO TO 108
000212          CALL SES(SESP,SOLEQS(1,I),1,FSP)
000221          FREENE(J)=FSP/R2T +FREENE(J)
000225          I=I+1
000227      107 CONTINUE
000231      110  GO TO 111
000232      108  IND=-2
000233          RETURN
000234      111 DO 112 I=1,NT
000236          XN1(I)=X(I)
000241      112 CONTINUE
000243          IND=0
000243          CALL EQUIL(AIK,X,FREENE,ELEM,M,N,NT,IND)
000254          IF(IND.EQ.-1) GO TO 113
000256          IF(IND.EQ.-7) RETURN
000260          AMOLER=0.
000261          DO114 I=1,NT
000263          AMOLER = AMOLER + ABS(X(I) - XN1(I))
000270      114 CONTINUE
000272          IF(AMOLER.LT.EXITME) RETURN
000274          GO TO 100
000275      113 IND=-3
000276          RETURN
000277          END
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                SUBROUTINE SYS2
          C     SYSTEM II        ASSUMES SYS1 JUST PERFORMED
000002           COMMON  X(25),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
               1FREENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
               2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,EO,IOEQ,ICJC,IHUG,IPVC,
               3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
               4ETOT,VTOT,VPG,ES(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
               5,VCJ,UCJ,CJT,CJS
000002           COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
               1,R3,R5,R6,SCALF,PO,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
               2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)
               3,ASBOS(10),ASBOSH(10),ASP(100),ASV(100),AST(100),ASE(100),ASG(100)
               4,ASUP(100),VAHX(2500),ALGV(100),CPRIME,DECIP,AMINP,AINCP,AMAXP
               5,ALX(101),FITP(100),FITT(100),FITE(100),PCOEF(5),TCOEF(5),ECOEF(5)
               6,W(100),DELY(100),SB(5),T(5),A(5,5),ALGP(100),DPDV(100),IT,IW
               7,ALGF(100),VBOS2,HUGH2,NSF,NAIK,VO
000002           EGT=0.
000003           DO 201 I=1,N
000005           CALL TDF(TEMP,THERC(1,I),1,HMHO)
000012           EGT=EGT+(X(I)/XBAR)*(HMHO-R1T*THERC(7,I))
000024      201 CONTINUE
000027           EGT=EGT+R1T*(ALPHA*TEMP*(FX-1.)/(TEMP+THETA))
000037           EST=0.
000037           VST=0.
000040           IF(N.EQ.NT) GO TO 202
000042           NS=N+1
000044           J=1
000045           DO 202 I=NS,NT
000047           CALL TDF(TEMP,THERC(1,I),1,HMHO)
000054           SESP(3) =VSOL(J)
000057           CALL SES(SESP,SOLEQS(1,J),2,ESP)
000064           ES(J)= HMHO +THERC(7,I)+ (R3)*(ESP)
```

```
000074          EST=EST +(X(I)*ES(J))
000101          VST=VST +(X(I)*VSOL(J)*SOLEQS(12,J))
000110          J=J+1
000111      202 CONTINUE
000114          ETOT=(XBAR)*(EGT)+EST
000117          VTOT=(XBAR)*(VGAS)+VST
000122          VPG =(VTOT)/AMOLWT
000124          RETURN
000124          END
```

```
                SUBROUTINE SYS2A (IND)
          C     SYSTEM II A  GIVEN P COMPUTE HUGONIOT TEMPERATURF
          C     IND IS -1 FOR VGAS LFR ERROR,-2 FOR VSOL LFB ERROR, -3 FOR EQUIL
          C     ERROR AND -4 FOR HUGONIOT TEMP LFB ERROR
000003          COMMON  X(25),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
               1FREENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
               2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,EO,IOEQ,ICJC,IHUG,IPVC,
               3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
               4ETOT,VTOT,VPG,ES(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
               5,VCJ,UCJ,CJT,CJS
000003          COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
               1,R3,R5,R6,SCALF,PO,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
               2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)
               3,ASBOS(10),ASBOSH(10),ASP(100),ASV(100),AST(100),ASE(100),ASG(100)
               4,ASUP(100),VAHX(2500),ALGV(100),CPRIME,DECIP,AMINP,AINCP,AMAXP
               5,ALX(101),FITP(100),FITT(100),FITE(100),PCOEF(5),TCOEF(5),ECOEF(5)
               6,W(100),DELY(100),SB(5),T(5),A(5,5),ALGP(100),DPDV(100),IT,IW
               7,ALGF(100),VBOS2,HUGB2,NSF,NAIK,VO
000003          DATA  SCALF/+1.0E-5/
000003          DATA  PO/+1.0E-6/
000003          DATA HUGB2 /+3.0E+3/
000003          DATA  HUGBOS(1)/+3.0E+3/
000003          DATA  HUGBOS(2)/+1.1/
000003          DATA  HUGBOS(3)/+1.0E-6/
000003          DATA  HUGBOS(10)/0./
000003      249 CALL LFB(TEMP,F,HUGBOS)
000007          IF(HUGBOS(10)) 250,252,251
000011      250 IND=-4
000012          RETURN
000013      251 CALL SYS1 (IND)
000015          IF(IND.LT.0)RETURN
000016          CALL SYS2
000020          F=(SCALF)*(ETOT-EO-(0.5)*(PRESS+PO)*(VO-VPG)*R3*AMOLWT)
000033          GO TO 249
000033      252 RETURN
000034          END
```

```
                SUBROUTINE SYS3(IND)
          C     SYSTEM III  FIND C-J VALUES
          C     ERRORS IND-1,VGAS LFB/-2, VSOL LFB/ -3, EQUIL/-4,HUG LFB/
          C     IND = -5 IF MIND ERROR
000003          COMMON  X(25),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
               1FREENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
               2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,EO,IOEQ,ICJC,IHUG,IPVC,
               3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
               4ETOT,VTOT,VPG,ES(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
               5,VCJ,UCJ,CJT,CJS
000003          COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
               1,R3,R5,R6,SCALF,PO,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
               2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)
```

```
                  3,ASBOS(10),ASBOSH(10),ASP(100),ASV(100),AST(100),ASE(100),ASG(100)
                  4,ASUP(100),VAHX(2500),ALGV(100),CPRIME,DECIP,AMINP,AINCP,AMAXP
                  5,ALX(101),FITP(100),FITT(100),FITE(100),PCOEF(5),TCOEF(5),ECOEF(5)
                  6,W(100),DELY(100),SB(5),T(5),A(5,5),ALGP(100),DPDV(100),IT,IW
                  7,ALGF(100),VBOS2,HUGB2,NSF,NAIK,VO
000003             DATA CJBOS(1)/0./
000003             DATA CJBOS(2)/+0.8/
000003             DATA CJBOS(3)/+1.0E-6/
000003             DATA CJBOS(4)/0./
000003             DATA APGCJ/+0.15/
000003             DATA BPGCJ/+0.25/
000003             CJBOS(1)= APGCJ + (BPGCJ)*(RHO-1.)
000007         300 CALL MIND (PRESS,DETVEL,CJBOS)
000013             IF (CJBOS(4))  310,311,312
000015         312 CALL SYS2A(IND)
000017             IF(IND.LT.0) RETURN
000020             DETVEL=(VO)*(SQRT((PRESS-PO)/( VO -VPG)))
000031             GO TO 300
000031         311 GAMMA=((RHO*((DETVEL)*(DETVEL)))/PRESS)-1.
000036             PCJ=PRESS
000037             VCJ= VPG
000040             CJT= TEMP
000042             UCJ= SQRT(PCJ*(VO-VPG))
000050             RETURN
000050         310 IND = -5
000051             RETURN
000052             END
```

```
                   SUBROUTINE SYS4
               C   SYSTEM 4  GIVEN P,T,V  CALCULATE  S  ASSUMES SYS1 HAS BEEN DONE
000002             COMMON  X(25),THFRC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
                  1FREENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
                  2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,EO,IOEQ,ICJC,IHUG,IPVC,
                  3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
                  4ETOT,VTOT,VPG,ES(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
                  5,VCJ,UCJ,CJT,CJS
000002             COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
                  1,R3,R5,R6,SCALF,PO,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
                  2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)
                  3,ASBOS(10),ASBOSH(10),ASP(100),ASV(100),AST(100),ASE(100),ASG(100)
                  4,ASUP(100),VAHX(2500),ALGV(100),CPRIME,DECIP,AMINP,AINCP,AMAXP
                  5,ALX(101),FITP(100),FITT(100),FITE(100),PCOEF(5),TCOEF(5),ECOEF(5)
                  6,W(100),DELY(100),SB(5),T(5),A(5,5),ALGP(100),DPDV(100),IT,IW
                  7,ALGF(100),VBOS2,HUGB2,NSF,NAIK,VO
000002             SPG= R1*( FGP+(ALPHA *TEMP*(FX-1.)/(TEMP+THETA)))-R1*ALNP
000013             SUM=0.
000014             DO 400 I=1,N
000015             SUM= SUM + (X(I)/XBAR)*ALOG(X(I)/XBAR)
000027         400 CONTINUE
000031             SPG= SPG -R1*SUM
000034             SUM=0.
000034             DO 401 I=1,N
000036             CALL TDF(TEMP,THERC(1,I),0,S(I))
000044             SUM =SUM +(X(I)/XBAR)*S(I)
000052         401 CONTINUE
000054             SGAS=SUM+SPG
000056             STOT=(XBAR)*(SGAS)
000057             IF(N.EQ.NT)  RETURN
000061             NS=N+1
000063             I=1
000064             DO 402 J=NS,NT
000066             CALL TDF(TEMP,THERC(1,J),0,S(J))
000074             SESP(3)= VSOL(I)
000077             CALL SES(SESP,SOLEQS(1,I),3,SS)
000104             S(J)= S(J) +(R3/R5)*SS
```

```
000111      402 CONTINUE
000113          SUM=0.
000114          DO 403 J=NS,NT
000116          SUM = SUM + (X(J))*(S(J))
000123      403 CONTINUE
000125          STOT = STOT + SUM
000127          RETURN
000127          END
```

```
                SUBROUTINE SYS4A (IND)
          C     SYSTEM 4A TO COMPUTF THE C-J ISENTROPE  IND =-6 FOR LFB S ERROR
000003          COMMON  X(25),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
               1FREENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
               2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,EO,IOEQ,ICJC,IHUG,IPVC,
               3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
               4ETOT,VTOT,VPG,ES(5).IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
               5,VCJ,UCJ,CJT,CJS
000003          COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
               1,R3,R5,R6,SCALF,PO,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
               2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)
               3,ASBOS(10),ASBOSH(10),ASP(100),ASV(100),AST(100),ASE(100),ASG(100)
               4,ASUP(100),VAHX(2500),ALGV(100),CPRIME,DECIP,AMINP,AINCP,AMAXP
               5,ALX(101),FITP(100),FITT(100),FITE(100),PCOEF(5),TCOEF(5),ECOEF(5)
               6,W(100),DELY(100),SB(5),T(5),A(5,5),ALGP(100),DPDV(100),IT,IW
               7,ALGF(100),VBOS2,HUGB2,NSF,NAIK,VO
000003          DATA CPRIME/+0.1/
000003          DATA DECIP/+0.7/
000003          DATA AMINP/+1.0E-4/
000003          DATA AINCP/+1.15/
000003          DATA AMAXP/+1.0/
000003          DATA ASBOS(2)/+0.9/
000003          DATA ASBOS(3)/+0.1/
000003          DATA ASBOS(10)/0./
000003          DATA ASBOSH(2)/+1.1/
000003          DATA ASBOSH(3)/+0.1/
000003          DATA ASBOSH(10)/0./
000003          VBOS=VBOS2
000005          PRESS=PCJ
000006          TEMP=CJT
000010          CALL SYS1 (IND)
000012          IF(IND.LT.0) RETURN
000013          CALL SYS4
000015          SCJ=STOT
000017          ASBOS=CJT
000020          ASBOSH=CJT
000021          I=1
000022          J=1
000023          CALL SYS2
000025          ASE(I)=(ETOT-EO)/(R3*AMOLWT) +CPRIME
000033          ASP(I)=PRESS
000035          ASV(I)=VPG
000037          AST(I)=TEMP
000041          DO 425 K=1,NT
000043          VAHX(J)=X(K)
000046          J=J+1
000050     425  CONTINUE
000052          I=I+1
000053      410 PRESS= PRESS*DECIP
000055          IF(PRESS.LT.AMINP) GO TO 450
000057      411 CALL LFB (TEMP,F,ASBOS)
000063          IF(ASBOS(10))  412,413,414
000065      412 IND = -6
000066          RETURN
000067      414 CALL SYS1(IND)
000071          IF(IND.LT.0) RETURN
000072          CALL SYS4
```

```
000074          F = STOT - SCJ
000076          GO TO 411
000077      413 CALL SYS2
000101          ASE(I)=(ETOT-EO)/(R3*AMOLWT) +CPRIME
000107          ASP(I)=PRESS
000111          ASV(I)=VPG
000113          AST(I)=TEMP
000115          DO 415 K=1,NT
000117          VAHX(J)=X(K)
000122          J=J+1
000124      415 CONTINUE
000126          I=I+1
000127          IF (I.GT.99) GO TO 470
000132          GO TO 410
000132      450 L=I-1
000134          PRESS = PCJ
000136          VBOS=VBOS2
000137      451 PRESS = PRESS* AINCP
000141          IF(PRESS.GT.AMAXP) GO TO 470
000144      452 CALL LFB (TEMP,F,ASBOSH)
000150          IF(ASBOSH(10)) 412,453,454
000152      454 CALL SYS1(IND)
000154          IF(IND.LT.0) RETURN
000155          CALL SYS4
000157          F = STOT - SCJ
000161          GO TO  452
000162      453 CALL SYS2
000164          ASE(I) =(ETOT-EO)/(R3*AMOLWT) + CPRIME
000172          ASP(I) = PRESS
000174          ASV(I) = VPG
000176          AST(I) = TEMP
000200          DO 455  K=1,NT
000202          VAHX(J)=X(K)
000205          J=J+1
000207      455 CONTINUE
000211          I=I+1
000212          IF (I.GT.99) GO TO 470
000215          GO TO 451
000215      470 I=I-1
000217          DO 471 K=1,I
000220          ALGV(K)=ALOG(ASV(K))
000226          ALGF(K)=ALOG(ASP(K))
000234      471 CONTINUE
000237          CALL PFTS(I,4,0,SIGMA,ALGV,ALGF,W,FITP,DELY,PCOEF,SB,T,ST,A)
000255          DO 472 K=1,I
000257          ALGF(K)=ALOG(AST(K))
000265      472 CONTINUE
000270          CALL PFTS(I,4,0,SIGMA,ALGV,ALGF,W,FITT,DELY,TCOEF,SB,T,ST,A)
000306          DO 473 K=1,I
000310          ALGF(K)=ALOG(ASE(K))
000316          ALGP(K)=ALOG(ASP(K))
000324      473 CONTINUE
000327          CALL PFTS(I,4,0,SIGMA,ALGP,ALGF,W,FITE,DELY,ECOEF,SB,T,ST,A)
000345          DO 474 K=1,I
000347          FITP(K)= EXP(FITP(K))
000355          FITT(K)= EXP(FITT(K))
000363          FITE(K)= EXP(FITE(K))
000371      474 CONTINUE
000374          DO 475 K=1,I
000375          AV=ALGV(K)
000377          ASG(K)=-PCOEF(2)-AV*(2.*PCOEF(3)+AV*(3.*PCOEF(4) +4.*AV*PCOEF(5)))
000413      475 CONTINUE
000415          ASUP=UCJ
000417          DO 480 K=2,L
000420          DELV=(ASV(K)-ASV(K-1))* 0.01
000424          ALX= ASV(K-1)
000426          DO 483 MZ=1,100
000430          ALX(MZ+1)=ALX(MZ)+DELV
000433      483 CONTINUE
000435          DO 481 MZ=1,101
```

```
000436            AV=ALOG(ALX(MZ))
000443            AP=EXP(PCOEF(1)+AV*(PCOEF(2)+AV*(PCOEF(3)+AV*(PCOEF(4)+ AV*PCOEF
                 1(5)))))
000457            DPDV(MZ)=SQRT(-(AP/ALX(MZ))*(PCOEF(2)+AV*(2.*PCOEF(3)+AV*(3.*PCOEF
                 1(4)+4.*AV*PCOEF(5)))))
000500        481 CONTINUE
000502            SUM=DPDV+ DPDV(101)+ 4.*DPDV(100)
000506            DO 482 MZ=2,98,2
000510            SUM= SUM + 4.*DPDV(MZ)+2.*DPDV(MZ+1)
000516        482 CONTINUE
000520            ASUP(K)=((DELV)/3.)*SUM    + ASUP(K-1)
000525        480 CONTINUE
000530            IW=L
000531            MZ=L+1
000533            DO 485 K=MZ,I
000534            ASUP(K)=0.
000536        485 CONTINUE
000540            IT=I
000541            RETURN
000541            END
```

```
                  SUBROUTINE SYS5 (IND)
            C     SYSTEM 5  TO COMPUTE HUGONIOT CURVE
000003            COMMON  X(25),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
                 1FREENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
                 2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,EO,IOEQ,ICJC,IHUG,IPVC,
                 3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
                 4ETOT,VTOT,VPG,ES(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
                 5,VCJ,UCJ,CJT,CJS
000003            COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
                 1,R3,R5,R6,SCALF,PO,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
                 2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)
                 3,ASBOS(10),ASBOSH(10),ASP(100),ASV(100),AST(100),ASE(100),ASG(100)
                 4,ASUP(100),VAHX(2500),ALGV(100),CPRIME,DECIP,AMINP,AINCP,AMAXP
                 5,ALX(101),FITP(100),FITT(100),FITE(100),PCOEF(5),TCOEF(5),ECOEF(5)
                 6,W(100),DELY(100),SR(5),T(5),A(5,5),ALGP(100),DPDV(100),IT,IW
                 7,ALGF(100),VBOS2,HUGB2,NSF,NAIK,VO
000003            DATA AMHUGP/+0.50/
000003            DATA DELP/+0.05/
000003            PRESS=AMHUGP
000005            I=1
000006            J=1
000007            VBOS=VBOS2
000010            HUGBOS=HUGB2
000012        500 CALL SYS2A(IND)
000014            IF (IND.LT.0) RETURN
000015            HUGP(I)=PRESS
000020            HUGT(I)=TEMP
000022            HUGV(I)=VPG
000024            IF(PRESS.LT.PCJ) GO TO 502
000026            IW=I
000027            HUGUS(I)=(VO)*(SQRT((PRESS-PO)/( VO -VPG)))
000040            DUP=SQRT((PRESS-PCJ)*(VCJ-VPG))
000047        501 HUGUP(I)= UCJ + DUP
000053        502 DO 503 K=1,NT
000055            VAHX(J)=X  (K)
000060            J=J+1
000062        503 CONTINUE
000064            PRESS=PRESS -DELP
000066            IF(PRESS.LT. DELP) RETURN
000067            I=I+1
000071            IT=I
000072            IF (I.GT.19) RETURN
000075            GO TO 500
000076            END
```

```
                    SUBROUTINE EQUIL (AIK,Y,FE,ELEM,NELE,NGAS,NTOT,IND)
              C     AIK IS ELEMENTAL SPECIE COMPOSITION MATRIX     NELE X NTOTAL DIMENSION
              C     Y IS NO MOLES OF EACH SPECIE                   NTOTAL DIMENSION
              C     FE IS FREE ENERGY OF EACH SPECIE               NTOTAL DIMENSION
              C     ELEM IS NO MOLES OF EACH ELEMENT               NELE DIMENSION
              C   NELE IS NO ELEMENTS
              C     NGAS IS NO GAS SPECIES
              C     NTOT IS TOTAL NO SPECIES
              C     IND IS -7 IF SINGULAR MATRIX AND -1 IF OTHER THAN LAST SOLID DISAPPEARED
 000011             DIMENSION AIK(250),Y(25),FE(25),ELEM(10),X(25),BMAT(36),AMAT(1296)
              C     THIS COMMON STATEMENT SPECIAL TO BKW CODE
 000011             COMMON/SUBVAR/AMAXE,AMINX,AMINY,TX(10)
 000011             DATA AMAXE/+1.0E-8/
 000011             DATA AMINX/+1.0E-11/
 000011             DATA AMINY/+1.0E-7/
 000011             SST=0.
 000012             DO 2 I=1,NTOT
 000013             IF(Y(I).LT.AMINY) Y(I)=AMINY
 000020           2 CONTINUE
 000023          35 NM1=NTOT+NELE+1
 000026             NN1=NTOT-NGAS
 000027             NM1SQ=NM1*NM1
              C     ZERO AMATRIX
 000031             DO 4 I=1,NM1SQ
 000033             AMAT(I)=0.
 000036           4 CONTINUE
              C     FORM SUMS
 000040             SUM=0.
 000041             DO 5 I=1,NGAS
 000042             SUM=SUM+Y(I)
 000045           5 CONTINUE
 000047             BARY=SUM
 000050             RBARY=(1.)/BARY
              C     FILL B MATRIX
 000051             I=1
 000052             DO 6 J=1,NGAS
 000054             BMAT(I)=-(FE(I)+ALOG(RBARY*Y(I)))
 000071             I=I+1
 000072           6 CONTINUE
 000075             IF(NN1.EQ.0) GO TO 7
 000076             DO 7 J=1,NN1
 000077             BMAT(I)=-(FE(I))
 000103             I=I+1
 000105           7 CONTINUE
 000110             DO 8 J=1,NELE
 000111             BMAT(I)=ELEM(J)
 000115             I=I+1
 000117           8 CONTINUE
 000121             BMAT(I)=0.
              C     FILL IN AMATRIX
 000124             I=1
 000125             DO 9 J=1,NGAS
 000127             AMAT(I)=(1.)/(Y(J))
 000134             I=I+NM1+1
 000137           9 CONTINUE
 000141             I=NTOT+1
 000143             J=1
 000144             L=1
 000145          12 DO 10 K=1,NELE
 000147             AMAT(I)=AIK(J)
 000154             I=I+1
 000155             J=J+1
 000156          10 CONTINUE
 000160             IF(L.GT.NGAS)GO TO 11
 000163             AMAT(I)=1.0
 000166          11 L=L+1
 000170             IF(L.GT.NTOT)GO TO 13
 000173             I=I+1+NTOT
 000174             GO TO 12
 000174          13 I=I+1
```

```
000176            DO 14 K=1,NGAS
000177            AMAT(I)=-RBARY
000203            I=I+1
000204         14 CONTINUE
000207            I=I+NN1+NELE
000211            AMAT(I)=-1.0
000214            I=I+1
000216            L=1
000217            J=1
000220         17 DO 15 K=1,NTOT
000222            AMAT(I)=AIK(J)
000227            J=J+NELE
000230            I=I+1
000232         15 CONTINUE
000235            I=I+NELE+1
000237            L=L+1
000240            IF(L.GT.NELE) GO TO 16
000242            J=L
000242            GO TO 17
000243        16  CALL LSS(NM1,1,NM1,AMAT,BMAT,D,DET,IND)
000257            IF(IND.LT.0) GO TO 40
         C        PUT ANSWERS IN X
000260            DO 18 I=1,NTOT
000262            X(I)=BMAT(I)
000266         18 CONTINUE
         C        TEST FOR TOO SMALL X
000271            DO 19 I=1,NGAS
000272            IF(X(I).LT.AMINX) X(I)=AMINX
000300         19 CONTINUE
         C        TEST TO SEE IF ANY SOLIDS DISAPPEARED
000303            IF(NN1.EQ.0) GO TO 20
000304            I=NGAS+1
000305            DO 20 J=1,NN1
000307            IF(X(I).LT.0.) GO TO 50
000311             I=I+1
000312         20 CONTINUE
         C        TEST TO SEE IF CONVERGED
000315            SUM=0.
000316            DO 21 I=1,NTOT
000317            SUM=SUM+ABS(Y(I)-X(I))
000325         21 CONTINUE
000327            IF(SUM.LT.AMAXE) GO TO 60
         C        RESOLVE WITH Y NOW HAVING LAST ANSWERS X
000331         31 DO 32 I=1,NTOT
000333            Y(I)=X(I)
000337         32 CONTINUE
000342            GO TO 35
         C        HAVE CONVERGED
000342         60 DO 38 I=1,NTOT
000344            Y(I)=X(I)
000350         38 CONTINUE
000353            J=NTOT+1
000355            IF(SST.LE.0.)GO TO 34
000356            Y(J)=0.
000361            NTOT=NTOT+1
000362         34 RETURN
         C        SOLID HAS DISAPPEARED
000363         50 SST=1.0
000365            IF(I.LT.NTOT)GO TO 33
000367            NTOT=NTOT-1
000370            GO TO 35
         C        AN ERROR HAS OCCURRED AS OTHER THAN LAST SOLID DISAPPEARED
         C        IND=-1 IF ERROR HAS OCCURRED
000371         33 IND=-1
000373            RETURN
         C        ERROR HAS OCCURRFD  MATRIX IS SINGULAR
000373         40 IND=-7
000375            RETURN
000375            END
```

```
               SUBROUTINE LFB (XP,FP,TX)
          C     TX(1)      INITIAL GUESS
          C     TX(2)      RATIO TO GET SECOND POINT
          C     TX(3)      ZERO DEFINITION
          C     TX(10)     COUNT OF NUMBER OF ITERATIONS
          C                SET TO ZERO ON SOLUTION
          C                SET TO NEGATIVE OF COUNT ON ERROR
          C     FP         =FUNCTION(XP)
          C     WHEN A SOLUTION IS FOUND, XP IS THE ROOT
          C
          C     ERROR EXITS OCCUR FOR
          C            1. TOO MANY ITERATIONS. .GT.CNTMAX
          C            2. TWO SUCESSIVE XP S OR FP S ARE EQUAL
000005         DIMENSION TX(10)
000005         DATA CNTMAX /1000./
000005         IF (TX(10).LE.0.) GO TO 1
000006         TX(10)=TX(10)+1.
000011         IF (TX(10)-3.) 2,3,4
          C  ENTRY FIRST TIME THROUGH
000014       1 IF (TX(1).EQ.0.) TX(1)=1.
000016         TX(10)=1.
000020         XP=TX(1)
          C  GO GET F(XP)
000021         RETURN
          C  ENTRY SECOND TIME THROUGH
000021       2 TX(9)=FP
000023         TX(8)=XP
000024         TX(5)=FP
000025         IF (ABS(FP).LT.TX(3)) GO TO 18
000027         XP=TX(1)*TX(2)
          C  GO GET F(XP)
000030         RETURN
          C  ENTRY THIRD TIME THROUGH
000031       3 TX(5)=FP
000033         TX(6)=XP
000034         TX(7)=FP
000035         IF (ABS(FP).LT.TX(3)) GO TO 18
000037         XP=TX(6)-TX(7)*(TX(6)-TX(8))/(TX(7)-TX(9))
          C  GO GET F(XP)
000046         RETURN
          C  ENTRY FOR FOURTH AND SUCEEDING TIMES THROUGH
000047       4 IF (TX(10).GT.CNTMAX) GO TO 99
000053         TX(4)=XP
000054         TX(5)=FP
000055         T=TX(4)-TX(6)
000057         IF (T.EQ.0.) GO TO 99
000060         IF (ABS(FP).LT.TX(3)) GO TO 18
000062         R=TX(5)-TX(7)
000064         IF (R.EQ.0.) GO TO 99
000065         XP=TX(4)-TX(5)*(T/R)
000071         IF (TX(5)*TX(7).LT.0.) GO TO 11
000073         IF (TX(5)*TX(9).GE.0.) GO TO 11
000075         IF (XP.GT.TX(4)) GO TO 6
000101         IF (XP.GT.TX(8)) GO TO 10
000104       8 XP=TX(4)-TX(5)*(TX(4)-TX(8))/(TX(5)-TX(9))
000113      10 TX(7)=TX(5)
000115         TX(6)=TX(4)
          C  GO GET F(XP)
000116         RETURN
000117       6 IF (XP.GT.TX(8)) GO TO 8
000123         GO TO 10
000123      11 TX(9)=TX(7)
000125         TX(8)=TX(6)
000126         GO TO 10
          C  HAVE FOUND A SOLUTION
000127      18 TX(10)=0.
000130         TX(1)=XP
000131         TX(4)=XP
000132         RETURN
          C  AN ERROR HAS OCCURED
```

```
        C  SET COUNT NEGATIVE AND EXIT
000133     99 TX(10)=-TX(10)
000135        RETURN
000135        END




                  SUBROUTINE MIND (P,D,PG)
        C         P CALCULATED
        C         D CALCULATED
        C         PG(1)=P GUESSED,PG(2)=RATIO NEXT TWO GUESSES,PG(3) MIN ERROR
        C         PG(4)=COUNT  SET TO ZERO ON SOLUTION
        C         COUNT IS SET EQUAL TO -1 IF GETS TOO BIG
000005            DIMENSION PG(4)
000005            DATA CNTMAX/1000./
000005            IF (PG(4).LE.0.)GO TO 1
000006            IF (PG(4).EQ.1.)GO TO 2
000010            IF (PG(4).EQ.2.)GO TO 3
000012            IF (PG(4).EQ.3.)GO TO 4
000014            IF (PG(4).GT.3.)GO TO 6
000017          1 P=PG(1)
000020            PG(4)=1.
000022            RETURN
000022          2 P3=P
000023            D3=D
000024            P=PG(1)*PG(2)
000026            PG(4)=2.
000027            RETURN
000030          3 P2=P
000031            D2=D
000032            P=P*PG(2)
000034            PG(4)=3.
000035            RETURN
000036          4 P1=P
000037            D1=D
000040            PG(4)=4.
000042          5 P=0.5*(P1*P1*(D3-D2)+P2*P2*(D1-D3)+P3*P3*(D2-D1))/
                 1(P1*(D3-D2)+P2*(D1-D3)+P3*(D2-D1))
000065            RETURN
000066          6 IF(D3.GT.D2) GOTO 7
000072            GO TO 8
000072          7 IF(D3.GT.D1) GO TO 9
000076            GO TO 10
000076          8 IF(D2.LT.D1) GO TO 10
000100            P2=P
000101            D2=D
000102            GO TO 11
000103          9 P3=P
000104            D3=D
000105            GO TO 11
000106         10 P1=P
000107            D1=D
000110            GO TO 11
000111         11 IF(ABS(D1-D2).LT.PG(3)) GO TO 12
000115            IF(ABS(D1-D3).LT.PG(3)) GO TO 12
000121            IF(ABS(D3-D2).LT.PG(3)) GO TO 12
000124            PG(4)=PG(4)+1.
000127            IF(PG(4).LT.CNTMAX)GO TO 5
000131            PG(4)=-1.
        C         ERROR HAS OCCURRED
000132            RETURN
000133         12 PG(4)=0.
000134            RETURN
000135            END
```

```
                   SUBROUTINE SES(P,A,IND,ANS)
             C     P,T,V  P,T INPUT TO FIND V AND P,T,V INPUT TO FIND F,E,OR S
             C     A-12 COEFF VO,A,B,C,D,E,A1,A2,C1,C2,C3,MOLWT
             C     IND, 0 FOR VOLUMF, 1 FOR F, 2 FOR E, 3 FOR S, SET TO -1 FOR ERROR
             C     ANS  F,E, OR S AND V IN ANS AND V
             C     IF A IS ZERO THEN INCOMPRESSIBLE SOLID
             C     THIS COMMON STATEMENT SPECIAL TO BKW CODE
             C     NEED TO PUT TX(10) IN DIMENSION STATEMENT IF REMOVE COMMON
000006             COMMON/SUBVAR/AMAXE,AMINX,AMINY,TX(10)
000006             DIMENSION P(3),A(12),       F(2),V(2)
000006             DATA TX(10)/0./
000006             DATA TX(2)/+1.1/
000006             DATA TX(3)/+1.0E-9/
000006             TV=P(2)/11605.6
000010             IF(IND.EQ.1) GO TO 10
000012             IF(IND.EQ.2) GO TO 20
000014             IF(IND.EQ.3) GO TO 30
             C     CALCULATE VOLUME
000016             IF (A(2).NE.0.) GO TO 1
000017             ANS=A(1)
000020             P(3)=A(1)
000021             RETURN
000021           1 TX(1)=TX(2)*1./A(1)
000024           5 CALL LFB(X,F,TX)
000032             IF(TX(10)) 2,4,3
000033           3 F=(A(2)+X*(A(3)+X*(A(4)+X*(A(5)+X*A(6)))))+
                  1(A(7)+A(8)*X)*TV +((A(9)+A(10)/X +A(11)/(X*X))*TV*TV)-P(1)
000062             GO TO 5
000063           4 P(3)=1./X
000065             ANS=P(3)
000066             RETURN
             C     ERROR IN ITERATION
000067           2 IND=-1
000070             RETURN
             C     CALCULATE FREE ENERGY
000071          10 IF (A(2).NE.0.)GO TO 11
000072             ANS=P(1)*A(1)*A(12)
000075             RETURN
000075          11 V(1)=P(3)
000077             V(2)=A(1)
000100             DO 12 I=1,2
000101             ALNV=ALOG(V(I))
000107             RHO =1./V(I)
000112             F(I)=(A(2)*V(I)+A(3)*ALNV-A(4)*RHO-A(5)*0.5*RHO*RHO
                  1-A(6)/3.*RHO**3 )+(A(7)*V(I)+A(8)*ALNV)*TV+(A(9)*V(I)+0.5*A(10)
                  2*V(I)*V(I)+A(11)/3.*V(I)**3 )*TV*TV
000156          12 CONTINUE
000160             ANS=A(12)*(P(1)*V(1)-(F(1)-F(2)))
000164             RETURN
             C     CALCULATE ENERGY
000164          20 IF(A(2).NE.0.)GO TO 21
000165             ANS=0.
000166             RETURN
000166          21 V(1)=P(3)
000170             V(2)=A(1)
000171             DO 22 I=1,2
000172             ALNV=ALOG(V(I))
000200             RHO=1./V(I)
000203             F(I)=(A(9)*V(I)+A(10)*V(I)*V(I)*0.5+A(11)*V(I)**3/3.)*TV*TV -
                  1(A(2)*V(I)+A(3)*ALNV-A(4)*RHO-A(5)*0.5*RHO*RHO-A(6)/3.*RHO**3 )
000242          22 CONTINUE
000244             ANS=A(12)*(F(1)-F(2))
000246             RETURN
             C     CALCULATE ENTROPY
000247          30 IF(A(2).NE.0.) GO TO 31
000250             ANS=0.
000251             RETURN
000251          31 V(1)=P(3)
000253             V(2)=A(1)
000254             DO 32 I=1,2
```

```
000255          ALNV=ALOG(V(I))
000263          F(I)=(A(7)*V(I)+A(8)*ALNV)+2.*TV*(A(9)*V(I)+0.5*V(I)*V(I)*A(10)+
               1A(11)/3.*V(I)**3 )
000306       32 CONTINUE
000310          ANS=A(12)*(F(1)-F(2))
000313          RETURN
000313          END
```

```
                SUBROUTINE  TDF   (T,A,IND,ANS)
         C      T  TEMPERATURE
         C      A  COEFFICIENTS  A,B,C,D,E,IC
         C      IND 0-FOR SO,1-FOR H-HO, 2-FOR F-HO/T WITH RESULT IN ANS
000006          DIMENSION A(6)
000006          IF(IND.EQ.1) GO TO 10
000010          IF(IND.EQ.2) GO TO 20
         C      CALCULATE SO
000012          ANS=A(1)+T*(A(2)+T*(A(3)+T*(A(4)+T*A(5))))
000022          RETURN
         C      CALCULATE H-H0
000022       10 ANS=A(6)+T*T *(0.5*A(2)+T*(2./3.*A(3)+T*(0.75 *A(4)+T*0.80 *A(5)))
               1)
000037          RETURN
         C      CALCULATE F-H0/T
000037       20 ANS=A(6)/T-(A(1)+T*(0.5*A(2)+T*(1./3.*A(3)+T*(0.25*A(4)+T*0.2  *
               1A(5)))))
000054          RETURN
000055          END
```

```
                SUBROUTINE LSS (N,M,I,A,B,D,DET,IND)
         C      SPECIAL VERSION OF LSS WITH IND ADDED AND INTERNAL ERROR PRINTS
         C      DELETED
         C      PURPOSE IS TO SOLVE MATRIX EQUATION AX = B
         C      N = NO ROWS A                M = NO COLUMNS IN B
         C      I = FIRST DIMENSION OF A(I,N)     B(I,M)
         C      A = ORIGIN OF NXN MATRIX A   B = ORIGIN OF NXM MATRIX B
         C      D  NOT USED           DET CONTAINS DETERMINANT OF A UPON RETURN
         C      IND = -7 IF MATRIX IS SINGULAR
         C      EACH ENTRY DESTROYS A, SOLUTIONS ARE IN B UPON RETURN
         C      A INVERSE IN B IF DET A NOT 0      IF M=0 ONLY DET A IS COMPUTED
000011          DIMENSION A(I,N),B(I,M),D(N)
000011          DOUBLE PRECISION S1,S2
000011          DIMENSION S1T(2),S2T(2)
000011          EQUIVALENCE (S1T,S1), (S2T,S2)
000011          NN = N
000012          MM = M
000013          X = 0.
000014          DO 1 J = 1,NN
000015          DO 1 K = 1,NN
000016          T = ABS(A(K,J))
000023          IF (T.GT.X) X = T
000026        1 CONTINUE
000033          IF (X.EQ.0.) GO TO 19
000034        2 SN = 1.
000036          DO 14 J = 1,NN
000037          L = J - 1
000041          IF (J.EQ.NN) GO TO 11
000043          T = ABS(A(J,J))
000047          M1 = J
000050          M2 = J + 1
000052          DO 3 K =M2,NN
```

```
000053          X = ABS(A(K,J))
000060          IF (X.LE.T) GO TO 3
000063          T = X
000063          M1 = K
000065        3 CONTINUE
000070          IF (M1.EQ.J) GO TO 6
000072          DO 4 K = 1,NN
000073          T = A(J,K)
000077          A(J,K) = A(M1,K)
000105        4 A(M1,K) = T
000114          DO 5 K = 1,MM
000115          T = B(J,K)
000121          B(J,K) = B(M1,K)
000127        5 B(M1,K) = T
000136          SN = -SN
000137        6 IF (A(J,J).EQ.0.) GO TO 19
000143          DO 10 K = M2,NN
000145          S1 = 0.
000147          S2 = 0.
000150          IF (L.EQ.0) GO TO 8
000151          DO 7 M3 = 1,L
000153        7 S1 = S1 + A(J,M3)*A(M3,K)
000177        8 A(J,K) =(A(J,K) - S1)/A(J,J)
000227          DO 9 M3 = 1,J
000230        9 S2 = S2 + A(K,M3)*A(M3,M2)
000254       10 A(K,M2) = A(K,M2) - S2
000267       11 DO 13 K = 1,MM
000271          S1 = 0.
000273          IF (L.EQ.0) GO TO 13
000274          DO 12 M3 = 1,L
000275       12 S1 = S1 + A(J,M3)*B(M3,K)
000321       13 B(J,K) = (B(J,K) - S1)/A(J,J)
000353       14 CONTINUE
000355          DET = A(1,1)*SN
000357          IF (DET.EQ.0.) GO TO 19
000360          IF (N.EQ.1) GO TO 21
000362          DO 15 J = 2,NN
000363       15 DET = DET*A(J,J)
000373          IF (DET.EQ.0.) GO TO 19
000374          IF (MM.EQ.0) GO TO 21
000375          M3 = NN-1
000377          DO 18 J = 1,MM
000400          DO 17 L = 1,M3
000401          M1 = NN - L
000403          S1 = 0.
000404          M2 = M1 + 1
000406          DO 16 K = M2,NN
000407       16 S1 = S1 +A(M1,K)*B(K,J)
000433       17 B(M1,J) = B(M1,J) - S1
000446       18 CONTINUE
000450          GO TO 21
           C    IF MATRIX IS SINGULAR ERROR EXIT OCCURS HERE
000451      19  IND=-7
000453       21 RETURN
000454          END




                SUBROUTINE   PFTS(M,KM,IW,SIGMA,X,F2,W,Y,DELY,B,SB,T,ST,A)
           C    THIS IS A SPECIAL VERSION OF LA-PFTS FOR A MAX OF 100 POINTS
           C    AND A MAX OF FIFTH DEGREE FIT  NO PRINTING  OR LEGENDRE POLYNOMIALS
           C    ALSO WILL COMPUTE TILL GET THE FIT AND REQUIRES NO OUTPUT SUBROUTINE
           C    M = NO OF DATA POINTS
           C    KM = DEGREE OF FIT  (MAX OF 5)
           C    IW = 0 FOR NO  WEIGHTS AND EQUAL 1 FOR WEIGHTS
           C    SIGMA       IS STANDARD DEVIATION COMPUTED
           C    X = X DATA       INPUT ARRAY
```

```
        C      F2 = F2 DATA ARRAY  INPUT
        C      W = WEIGHT DATA ARRAY  INPUT    SET EQUAL TO 1 IF IW IS 0
        C      Y  =  F COMPUTED FROM FIT USING X
        C      DELY = DIFFERENCE IN COMPUTED AND INPUT F
        C      B = COEFFICIENTS TO FIT
        C      SB = ESTIMATE OF ERRORS IN COEFFICIENTS TO FIT
        C      T = COEFFICIENTS TO ORTHOGONAL POLYNOMINALS
        C      ST = ERRORS IN T
        C      A = AREA USED BY CALCULATION
000017         DIMENSION   S(5),X(100),F2(100),ST(5),SB(5),F(100),PM(100),P(100)
              1 , B(5),DELY(100),W(100),A(5,5),T(5),Y(100)
000017         LL=0
000020       9 FM=0.0
000021         A(1,1)=1.0
000024         A(2,2)=1.0
000026         FBAR=0.0
000027         XBAR=0.0
000030         DO10I=1,M
000031         IF(IW)1009,1010,1009
000032    1010 W2=1.0
000034         W(I)=1.0
000037         GOTO1011
000040    1009 W2=SQRT(W(I))
000051    1011 FM=FM+W(I)
000055         F(I)=W2*F2(I)
000061         PM(I) = W2
000064         FBAR=FBAR+F(I)*PM(I)
000071      10 XBAR=XBAR+X(I)*PM(I)**2
000077         XBAR=XBAR/FM
000100         T(1)=FBAR/FM
000103         A(2,1)=-XBAR
000106         PXF=0.0
000107         PXP=0.0
000110         DO20I=1,M
000111         P(I)=(X(I)-XBAR)*PM(I)
000117         PXF=PXF+P(I)*F(I)
000124      20 PXP=PXP+P(I)*P(I)
000131         T(2)=PXF/PXP
000134         PMXPM=FM
000136         S(1)=PMXPM
000137         KM=KM+1
000140         B(1)=T(1)*A(1,1)+T(2)*A(2,1)
000147         B(2)=T(2)*A(2,2)
000154      60 DO190K=2,KM
000156         IF(K-2)40,165,65
000160     40  STOP
000162      65 XPXP=0.0
000163         XPXPM=0.0
000164         B(K)=0.0
000167         DO70J=1,M
000171         XP=X(J)*P(J)
000175         XPXP=XPXP+XP*P(J)
000200      70 XPXPM=XPXPM+XP*PM(J)
000205         ALPHA=XPXP/PXP
000207         BETA=XPXPM/PMXPM
000211         PPXF=0.0
000212         PPXPP=0.0
000213         DO90I=1,M
000214      80 PT=P(I)
000217      81 P(I)=X(I)*PT-ALPHA*PT-BETA*PM(I)
000230      82 PPXF=PPXF+P(I)*F(I)
000235      83 PPXPP=PPXPP+P(I)*P(I)
000241      90 PM(I)=PT
000246         T(K)=PPXF/PPXPP
000252         PMXPM=PXP
000254         PXP=PPXPP
000254         A(K,1)=-ALPHA*A(K-1,1)-BETA*A(K-2,1)
000264         A(K,K-1)=A(K-1,K-2)-A(K-1,K-1)*ALPHA
000276         A(K,K)=1.0
000302         IF(K-3)150,150,110
```

```
000304      110 K1=K-2
000306          DO120I=2,K1
000310      120 A(K,I)=A(K-1,I-1)-ALPHA*A(K-1,I)-BETA*A(K-2,I)
000342      150 DO160I=1,K
000344      160 B(I)=B(I)+T(K)*A(K,I)
000364      165 SIG2=0.0
000365          DO180I=1,M
000367          Y(I)=POLY (X(I),K,B)
000404      175 DELY(I)=Y(I)-F2(I)
000413      180 SIG2=SIG2+(DELY(I)**2)*W(I)
000423          SIG2=SIG2/FLOAT(M-K;
000426          SIGMA=SQRT(SIG2)
000433          S(K) = PXP
000437          DO499I=1,K
000441      499 ST(I)=SIGMA/SQRT(S(I))
000457          DO501I=1,K
000461          SB(I)=0.0
000464          DO500J=I,K
000465      500 SB(I)=SB(I)+(A(J,I)*ST(J))**2
000507      501 SB(I)=SQRT(SB(I))
000522      190 CONTINUE
000524      220 KM=KM-1
000526          RETURN
000526           END
```

```
                FUNCTION POLY  (X,N,A)
000005          DIMENSIONA(2)
000005          Y=A(N)
000007          DO1I=2,N
000010          J=N-I+1
000012        1 Y=A(J)+Y*X
000020          POLY  =Y
000021          RETURN
000022          END
```

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