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

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

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 HOM⁴ 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 $^{\circ}\text{K}$
P	Pressure in Mbar
SO or S°	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
$(\Delta H_f^{\circ})_i$	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/usec
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 I2A6)
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 $SO \text{ (cal/mole-}^\circ K) = A + BT + CT^2 + DT^3 + ET^4$

No. 6 Then the integration constant from

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

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 V_0 (cc/g)

Nos. 2-11 If V_0 (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:

$A_s, B_s, C_s, D_s, E_s, A_1, A_2, C_1, C_2, C_3$

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

	C	H	N	O
H ₂ O	0	2	0	1
H ₂	0	2	0	0
O ₂	0	0	0	2
	etc.			

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 $> 0 \leq 4$, that number of densities are read and the re-

quested 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 $> 0 \leq 25$, 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.

PROGRAMMER: MADER				LOADING FORM				DATE:				PAGE 1 OF 3					
1		5		9		33		37		51		55		59		73	
X.XX		X.XX		X.XX		X.XX		X.XX		X.XX		X.XX		X.XX		CARD NO.	
0000 0001 0001 0001 0000 0000 0000 0000		0001 0001 0000 0000 0000 0000 0000 0000		0000 0000 0000 0000 0000 0000 0000 0000		0000 0000 0000 0000 0000 0000 0000 0000		0000 0000 0000 0000 0000 0000 0000 0000		0000 0000 0000 0000 0000 0000 0000 0000		0000 0000 0000 0000 0000 0000 0000 0000		0000 0000 0000 0000 0000 0000 0000 0000		1	
RDX		C.Y.C.L.O		T.R.I.M.E.T.H.Y.L.E.N.E		T.R.I.N.I		T.R.A.M.I.N.E								2	
0004 0011 0012																3	
+0.5		+000+1.6				-001+4.0				+002+1.09		097784436		+001		4	
C		H		N		M										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		O2		C2		NH3		H		N2		CH4		9	
S01 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+1.480805				-002-2.639181				-006+1.920453				-010		14	
+0.0		+000+1.34282835156				+003-5.7107				+004+3.46				+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+2.47703				-010		20	
+0.0		+000+7.46280968750				+002+9.3968				+004+6.70				+002		21	
+4.533082		+001+1.228161				-002-2.416403				-006+1.828181				-010		22	
+0.0		+000+1.12158830990				+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	

IV. FORTTRAN BKW OUTPUT. 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 CYCLOTETRAMETHYLENE 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= 5.0000000000E-01 BETA= 1.6000000000E-01 THE TA= 4.6000000000E+02 KAPPA= 1.09097784436E+01

THE COMPOSITION OF THE EXPLOSIVE IS

3.0000000000E+00 MOLES OF C
6.0000000000E+00 MOLES OF H
6.0000000000E+00 MOLES OF N
6.0000000000E+00 MOLES OF O

THE DENSITY OF THE EXPLOSIVE IS 1.8000000000E+00, GRAMS/CC

THE MOLECULAR WEIGHT IS 2.2212600000E+02 GRAMS

THE HEAT OF FORMATION AT 0 DEG K IS 3.3970000000E+04 CALORIES PER FORMULA WEIGHT

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

SOL C 4.4444444444E-01 8.3093583726E-01 -1.3938180921E+00 6.72569716021E-01 -1.1353726250E-01 6.49155882007E-03
-2.2670534594E-01 1.20516569525E-01 8.3160000000E-02 -1.7559000000E-01 1.5531000000E-01 1.2010000000E+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 CYCLOTTRIMETHYLENE 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
N2O	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	1.48906096265E+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	2.95040784085E-05	4.20181600000E+01 1.91166200000E-02 -3.16433000000E-06 2.19780100000E-10 0.
		1.20696121615E+03 -9.36800000000E+03 4.76000000000E+02
H	5.9637876225E-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 2.47671400000E-10 0.
		1.04242791146E+03 -1.60000000000E+04 5.28000000000E+02
SOL C	1.48906128705E+00	-2.46151900000E-01 7.17985500000E-03 -1.29755000000E-06 9.34995000000E-11 0.
		-2.58204389323E+02 0. 0.

THE BKW HUGONIOT FOR THE DETONATION PRODUCTS OF
RDX CYCLOTRIMETHYLENE TRINITRAMINE

PRESSURE = 5.0000000000E-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
N	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 = 4.5000000000E-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/MICROSECOND

SPECIE	NO OF MOLES
H2O	2.99998078763E+00
H2	2.52522105824E-06
O2	1.35656509186E-05
CO2	1.49266608115E+00
CO	1.44776503827E-02
NH3	1.10252722769E-05
N	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 = 4.0000000000E-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
N	4.83313590782E-10
NO	1.14178952130E-04
N2	2.99993470567E+00
OH	4.31442574033E-10
CH4	1.41845803046E-07
SOL C	1.49164552500E+00

PRESSURE = 3.5000000000E-01 VOLUME = 4.14600769335E-01 TEMPERATURE = 2.59153062904E+03
SHOCK VELOCITY = 8.73429108468E-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
N	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 = 3.0000000000E-01 VOLUME = 4.36835280098E-01 TEMPERATURE = 2.54370083879E+03

SPECIE	NO OF MOLES
H2O	2.99988911914E+00
H2	2.29785316955E-05
O2	1.56725927136E-06
CO2	1.48474001089E+00
CO	3.05726923301E-02
NH3	5.72203253117E-25
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
H2O	2.99971100941E+00
H2	7.50244687743E-05
O2	9.02931899893E-07
CO2	1.47517781751E+00
CO	4.58868112398E-02
NH3	1.37051733754E-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
H2O	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
H2O	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	4.4324220272E-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
H2O	2.97504092530E+00
H2	1.38668066707E-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

A BKW ISENTROPE THRU BKW CJ PRESSURE FOR
RDx CYCLOTRIME THYLENE TRINITRAMINE

LN(P)= -3.49297740731E+00 -2.54806028626E+00LNv 2.56284384201E-01LNv2 9.74735285967E-03LNv3 -9.36201089664E-03LNv4

LN(T)= 7.41443241083E+00 -4.90817152634E-01LNv 3.75181959834E-02LNv2 2.84869451321E-02LNv3 -9.96133737672E-03LNv4

LN(E)= -1.60502412233E+00 5.19208252102E-01LNv 6.59353610896E-02LNv2 4.07879169323E-03LNv3 9.83423378158E-03LNv4

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	4.15933350982E-01	2.58759366556E+03	1.24200627104E-01	2.94991700019E+00	2.20002528743E-01
2.42663854147E-01	4.69093987956E-01	2.44025410622E+03	1.08763295438E-01	2.90305348376E+00	2.93278938450E-01
1.69864697903E-01	5.29059666043E+03	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+00	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	5.78953120300E-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	2.30636211859E+00	7.06571279570E-01
6.85463326234E-03	1.86879462348E+00	1.24721284584E+03	4.98564394379E-02	2.2527636309E+00	7.35051238503E-01
4.79825728364E-03	2.20386399502E+00	1.16962429208E+03	4.79361788042E-02	2.14324065525E+00	7.61291260795E-01
3.35878008855E-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	8.83378800273E-01
3.95157119814E-04	8.27415256663E+00	7.40475883596E+02	4.00656452946E-02	1.68771205200E+00	8.99476598168E-01
2.7660998387E-04	1.02313668969E+01	6.88201867397E+02	3.94216420729E-02	1.66889738003E+00	9.14708556278E-01
1.93626988705E-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	9.42862453783E-01
9.98662046098E-05	3.96885356962E-01	2.64297698676E+03	1.31281189881E-01	2.96720442086E+00	0.
4.58461353013E-01	3.78694889350E-01	2.69633703138E+03	1.39060223226E-01	2.98391886698E+00	0.
5.27230555965E-01	3.1228541397E-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	3.0328242827E+00	0.
8.01851771804E-01	3.11225320419E-01	2.88721210089E+03	1.80250775357E-01	3.04695587055E+00	0.
9.22129537574E-01	2.97898690227E-01	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	3.42087052513E-01	2.58759366556E+03	2.56248322413E+03	1.24200627104E-01	1.24207807428E-01
2.42663854147E-01	2.40586891593E-01	2.44025410622E+03	2.42074102090E+03	1.08763295438E-01	1.08692586084E-01
1.69864697903E-01	1.69348084478E-01	2.29059666043E+03	2.28081441187E+03	9.63895994894E-02	9.63283656078E-02
1.18905288532E-01	1.19157824052E-01	2.14384498360E+03	2.14374764316E+03	8.63993698681E-02	8.63780985501E-02
8.32337019724E-02	8.3275002576E-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	7.16866602178E-02
4.07845139665E-02	4.11975746634E-02	1.74509810113E+03	1.75935749854E+03	6.61902223966E-02	6.62354393554E-02
2.85491597765E-02	2.88350791677E-02	1.62857115419E+03	1.64284108478E+03	6.14438841083E-02	6.17133088676E-02
1.99844118436E-02	2.01552733611E-02	1.52077981649E+03	1.53302234751E+03	5.78953120300E-02	5.78368855460E-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
6.85463326234E-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	1.16465822206E+03	4.79361788042E-02	4.79075057165E-02
3.35878008855E-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	1.63242289053E-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	4.08142553007E-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	3.94383963074E-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
9.98662046098E-05	9.92996643917E-05	2.64297698676E+03	2.61033667923E+03	1.31281189881E-01	1.31355575861E-01
4.58461353013E-01	4.51875509384E-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	6.07199600712E-01	2.79504209255E+03	2.78813873069E+03	1.57283774060E-01	1.57424348318E-01
6.97262410264E-01	6.97308127395E-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
9.22129537574E-01	9.33448003657E-01	2.90313821785E+03	2.95666916073E+03	1.91682860924E-01	1.92687622960E-01

THE ISENTROPE PRESSURE AND COMPOSITION OF DETONATION PRODUCTS												SOL C		
M20	H2	O2	CO2	CO	NH3	H	NO	N2	OH	CH4				
3.46662648781E-01				2.99994536397E+00				9.45374836410E-06				2.88697880055E-06	1.48906096240E+00	2.18525889737E-02
2.95040751845E-03				5.39687882169E-10				7.41458034516E-05				2.99994617506E+00	4.96489084344E-10	3.61824334079E-07
1.48908608690E+00														
2.42663854147E-01				2.99976043518E+00				6.09941217255E-05				5.21332382729E-07	1.47916778172E+00	4.18738838230E-02
1.14736428427E-04				5.07547218878E-08				2.90291441216E-05				2.99992810721E+00	4.5758668323E-08	3.19390071299E-06
1.47895514056E+00														
1.69864697803E-01				2.99920373220E+00				2.72662825546E-04				8.99891545333E-08	1.46611943938E+00	6.85467598778E-02
3.25021707223E-04				9.89322586324E-08				1.03468345323E-05				2.99983231573E+00	1.02356137151E-07	1.79858850558E-05
1.46531581486E+00														
1.18905288332E-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														
8.32337019724E-02				2.99468942998E+00				2.60381197673E-03				2.83910839781E-10	1.43550724713E+00	1.34294911952E-01
1.44688203107E-03				1.66675128540E-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	1.66621691184E-07	8.02372271088E-04
1.41066408473E+00														
4.07845139685E-02				2.97766739078E+00				1.23606457337E-02				2.88706525368E-11	1.41568940004E+00	1.90955468223E-01
3.82556219651E-03				1.17939826750E-07				6.09579170639E-08				2.99808718842E+00	1.19901545931E-07	2.1167506345E-03
1.39123930111E+00														
2.85491597785E-02				2.95976403777E+00				2.21834839588E-02				1.00000000000E-11	1.41667736755E+00	2.06881555101E-01
5.39766330350E-03				7.66791362799E-08				4.99134882360E-10				2.995730116810E+00	7.13431657530E-08	4.97795460571E-03
1.37146352275E+00														
1.99844118436E-02				2.93278309903E+00				3.56956363010E-02				1.00000000000E-11	1.42783967649E+00	2.11537543844E-01
7.01966834889E-03				4.28146017494E-08				9.79528923684E-10				2.99649016534E+00	3.22842464918E-09	1.04958695630E-02
1.35012681011E+00														
1.39890882905E-02				2.89484774473E+00				5.23704420272E-02				1.00000000000E-11	1.44953508591E+00	2.06082082868E-01
8.50070008388E-03				5.62951057002E-10				1.64461109263E-10				2.99574964988E+00	5.24590383375E-10	2.00153812887E-02
1.324367444994E+00														
9.79236180335E-03				2.84665908778E+00				7.01219022697E-02				1.00000000000E-11	1.48181981471E+00	1.89701282469E-01
9.9251767251E-03				4.50135618947E-10				6.45287598391E-11				2.99520374113E+00	4.03011766757E-10	3.44151165060E-02
1.29406378631E+00														
6.85465326234E-03				2.79088078573E+00				8.6822925139E-02				1.00000000000E-11	1.52206006849E+00	1.65799077189E-01
1.01824234516E-02				3.37342668808E-10				1.43610661539E-11				2.99490878827E+00	2.86129996312E-10	5.39116431356E-02
1.25822921118E+00														
4.79825728364E-03				2.72902711265E+00				1.00304028700E-01				1.00000000000E-11	1.56671501376E+00	1.37542859907E-01
1.02463923344E-02				2.31363103806E-10				1.00000000000E-11				2.99487680384E+00	1.81437431171E-10	7.76496349659E-02
1.21809249137E+00														
3.35878009855E-03				2.66846045761E+00				1.08873611840E-01				1.00000000000E-11	1.61171877107E+00	1.08101960489E-01
9.85068572387E-03				1.38874295967E-10				1.00000000000E-11				2.99507465715E+00	9.60672234168E-11	1.03894930921E-01
1.17628433752E+00														
2.35114606898E-03				2.61337276854E+00				1.12014974913E-01				1.00000000000E-11	1.65321516726E+00	8.01968973187E-02
9.11135934040E-03				6.65804427379E-11				1.00000000000E-11				2.99544432035E+00	3.68004725379E-11	1.30472608740E-01
1.13611532668E+00														
1.64580224829E-03				2.56797782667E+00				1.09357988044E-01				1.00000000000E-11	1.68809486375E+00	5.8324463132E-02
8.15346936067E-03				2.10860153377E-11				1.00000000000E-11				2.99592326535E+00	1.00000000000E-11	1.55216990614E-01
1.10085569932E+00														
1.15208157380E-03				2.53531654586E+00				1.01546057386E-01				1.00000000000E-11	1.71424941124E+00	3.61846322673E-02
7.08543980527E-03				1.00000000000E-11				1.00000000000E-11				2.99645728014E+00	1.00000000000E-11	1.76254618527E-01
1.07331133797E+00														
8.06443101661E-04				2.51839932658E+00				8.91094285167E-02				1.00000000000E-11	1.73010969561E+00	2.13812829160E-02
5.97636011257E-03				1.00000000000E-11				1.00000000000E-11				2.99701182000E+00	1.00000000000E-11	1.91763352378E-01
1.05674566909E+00														
5.64510171163E-04				2.51528238704E+00				7.45538633081E-02				1.00000000000E-11	1.73653933629E+00	1.16389412282E-02
4.91669365689E-03				1.00000000000E-11				1.00000000000E-11				2.99754165325E+00	1.00000000000E-11	2.91394354606E-01
1.05042736787E+00														
3.95137119814E-04				2.52743775000E+00				5.87362128859E-02				1.00000000000E-11	1.73344431076E+00	5.67362946170E-03
3.92602733135E-03				1.00000000000E-11				1.00000000000E-11				2.99803698642E+00	1.00000000000E-11	2.03968498090E-01
1.05691356169E+00														
2.76609983870E-04				2.55414103669E+00				4.32005967167E-02				1.00000000000E-11	1.72171557855E+00	2.42780736848E-03
3.03048051031E-03				1.00000000000E-11				1.00000000000E-11				2.99848475985E+00	1.00000000000E-11	1.99036322962E-01
1.07680028112E+00														
1.93626888708E-04				2.59487678542E+00				2.93065347811E-02				1.00000000000E-11	1.70281712597E+00	8.88963970201E-04
2.24712297497E-03				1.00000000000E-11				1.00000000000E-11				2.99887643864E+00	1.00000000000E-11	1.86622997731E-01
1.10897091233E+00														
1.35538892086E-04				2.64534086740E+00				1.80290883138E-02				1.00000000000E-11	1.67719494386E+00	2.69246417138E-01
1.58623275859E-03				1.00000000000E-11				1.00000000000E-11				2.99920688377E+00	1.00000000000E-11	1.67125387653E-04
1.15541042207E+00														
3.88682046088E-01				2.99997274773E+00				3.98516351993E-06				5.67873640102E-06	1.49187285864E+00	1.59652551438E-02
1.53403686889E-05				4.68404520002E-10				1.04921951486E-04				2.99993988884E+00	4.15578670041E-10	1.20054108183E-07
1.49208175816E+00														
4.58461353013E-01				2.99998745637E+00				1.52899272190E-06				1.13781337723E-05	1.49433590577E+00	1.11703035283E-02
7.28893407541E-06				3.41426883942E-09				1.47669983977E-04				2.99992252054E+00	2.30424004397E-09	3.91876626369E-08
1.49449375151E+00														
5.2723055865E-01				2.99999482993E+00				5.23964022729E-07				2.35992522204E-05	1.49617324215E+00	7.40344373562E-03
3.08660481242E-06				3.13436183813E-10				2.08043281199E-04				2.99989443006E+00	2.48897530106E-10	4.60941711583E-10
1.49642331385E+00														
6.06315139360E-01				2.99998812523E+00				1.57103275424E-07				5.22837324560E-05	1.49750776663E+00	4.58377447719E-03
1.14460689152E-08				2.34228300448E-10				2.97999482457E-04				2.99885048800E+00	1.70888323418E-10	1.70888323418E-10
1.49790845861E+00														
6.97262410244E-01				2.99999941423E+00				4.14726663687E-08				1.36567323013E-04	1.49831867825E+00	2.62774992294E-03
3.62389821288E-07				3.44356328909E-10				4.62344527808E-04				2.99976864654E+00	1.78527990648E-10	2.23979217812E-10
1.49905357181E+00														
8.01851771804E-01				2.99999987552E+00				4.36136042792E-10

V. FORTTRAN 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} .

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

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

$$c. 0 = F(x) - \frac{PV_g}{R_2 T}.$$

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

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

b. Form

$$F_i^* = \left(\frac{F-HO}{R_1 T} \right)_i + \frac{(\Delta H_f^0)_i}{R_1 T} + \ln(R_4 \cdot P) - \left[\ln F(x) - \left(\frac{e^{\beta W} - 1}{\beta} \right) - Kk_i \frac{F(x)^{-1}}{Z} \right].$$

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 .

$$(G^*)_i = \left(\frac{F-HO}{R_1 T} \right)_i + \frac{(\Delta H_f^0)_i}{R_1 T} + \frac{F'_s}{R_2 T}.$$

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.

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

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

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

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} .

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

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

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).

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

0.15 is in APCCJ, 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.

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

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

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

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

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

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

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

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

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

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

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

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.

$$E' = (E_{\text{Total}} - E_0) / [(R_3)(\text{AMOLWT})] + \text{CPRIME}.$$

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

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

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

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

Simpson's rule is

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

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

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

1. $P = \text{AMHUGP} - (n)(\text{DELP})$ 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. $U_s = V_0' \left(\frac{P}{V_0' - \text{VPG}} \right)^{\frac{1}{2}}$ computed if $P > P_{CJ}$.
4. $U_p = (U_p)_{CJ} + (P - P_{CJ})(V_{CJ} - \text{VPG})$ 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	EXITIME	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

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

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

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

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

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

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

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

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

The Matrix $[A]X = [B]$

	1	N	N+1	NT	1	M			
1	$\frac{1}{\bar{Y}_1}$			$\frac{1}{\bar{Y}}$	$\frac{1}{\bar{Y}_1}$		X_1	1	$-f_1(y)$
	$\frac{1}{\bar{Y}_2}$			$\frac{1}{\bar{Y}}$					
	$\frac{1}{\bar{Y}_N}$			$\frac{1}{\bar{Y}}$					
N									
N+1									
NT							X_{NT}	NT	$-G_1^0$
1							$\bar{X}$	1	
							π_1		b_k
							π_M	M	
M									
	1	1	1	0	-1	0			
	X_1				$\bar{X}$	π_k			

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

The Constraints

1. The initial Y_1 may not be smaller than 1×10^{-7} (AMINY).
2. The X_1 for $i = 1$ to N may not be smaller than 1×10^{-11} (AMINX).
3. The X_1 for $i = N+1$ to 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 $\sum_{i=1}^{NT} |Y_i - X_i| < 1 \times 10^{-8}$ (AMAXE).
5. Otherwise X_1 for $i = 1$ to NT to 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 MKW, 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, $C_4H_8N_8O_8$

$\downarrow$ k
 i

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

$$F^* = \frac{\mu_i}{RT} - \ln X_i = \left(\frac{F^{\circ} - H^{\circ}}{RT} \right)_i + \left(\frac{AH_f^{\circ}}{RT} \right)_i + \ln P$$

+ 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. FORTTRAN 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 $|FN2| < \text{max zero}$, 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 $|FN1| < \text{max zero}$, 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. FORTTRAN 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.

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

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

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

$$\frac{F-HO}{T} = - \left(A + \frac{BT}{2} + \frac{CT^2}{3} + \frac{DT^3}{4} + \frac{ET^4}{5} \right) + \frac{IC}{T},$$

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

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. FORTTRAN 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

$\rho_{\text{guessed}} = 1.1 [TX(2)] \rho_o$, 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, $F'_s = (P)(V_o)(\text{MOLWT})$,

b.

$$F'_s = (\text{MOLWT}) \left\{ PV_s - \left[\left(A_s V_s + B_s \ln V_s - \frac{C_s}{V_s} - \frac{D_s}{2V_s^2} - \frac{E_s}{3V_s^3} \right) \right. \right. \\ \left. \left. + \left(A1V_s + A2 \ln V_s \right) T_v + \left(C1V_s + \frac{C2V_s^2}{2} + \frac{C3V_s^3}{3} \right) T_v^2 \right] \right\} V_o$$

Units are Mbar-cc/mole.

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

a. If incompressible, $E'_s = 0$,

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

Units are Mbar-cc/mole.

4. To find the imperfection entropy (S'_s):

a. If incompressible, $S'_s = 0$,

$$b. S'_s = (\text{MOLWT}) \left[(A1V_s + A2 \ln V_s) + 2T_v \right.$$

$$\left. \left(C1V_s + \frac{C2V_s^2}{2} + \frac{C3V_s^3}{3} \right) \right] V_o$$

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 ($^{\circ}$ K),
P(3) volume (cc/g for imperfec-
tion 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 en-
ergy, 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

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

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 mini-
mum is reached,
PG(4) Cycle count - set to ze-
ro 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.

```

000003      PROGRAM BKW (INPUT,OUTPUT,FILM,TAPE12=FILM)
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,E0,IOEQ,ICJC,IHUG,IPVC,
3IGRP,IDIC,IRHO,IONL,IMIS,IEXT,FX,RIT,R2T,XBAR,
4ETOT,VTOT,VP,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,P0,HUGBOS(10),CJBOS(4),APGCJ,HPGCJ
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),FCOEF(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 ATRHO(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,E0
000135      READ 902, TEMP,PRESS

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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 EXIME=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

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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(115.1E18.11)
001113      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 IDENTITY NO .115. 4H IS .1PE18.11)
001113      END

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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/ VBO5(10),EXITME,SESP(3),R1,R2,ABTOA
1,R3,R5,R6,SCALF,PO,HUGHOS(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),VROS2,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)

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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
15/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,1PE7.1))
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

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000002 C      SUBROUTINE HUGPNT
      THE PRINTING AND GRAPHING OF HUGONIOT RESULTS
      COMMON X(25),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
1FREENE(25),XN1(25),VSOL(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,VPGE,S(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
5,VCJ,UCJ,CJT,CJS
000002      COMMON / RST/ VBOS(10),EXITIME,SESP(3),R1,R2,ABTOA
1,R3,R5,R6,SCALF,P0,HUGBOS(10),CJROS(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

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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) RETURN
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 PRESSURE 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

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          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,E0,IOEQ,ICJC,IHUG,IPVC,
          3IGRP,IDIC,IRHO,I0NL,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,P0,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
          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 TEMPERATURE 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 RKW ISENTROPE THRU BKW CJ PRESSURE FOR )
000662      903 FORMAT(//,8H LN(P)= ,1PE18.11,3X,1PE18.11,5HNLV ,1PE18.11,6HNLV*2
000662      1 ,1PE18.11,6HNLV*3 ,1PE18.11,5HNLV*4)
000662      904 FORMAT(//,8H LN(T)= ,1PE18.11,3X,1PE18.11,5HNLV ,1PE18.11,6HNLV*2
000662      1 ,1PE18.11,6HNLV*3 ,1PE18.11,5HNLV*4)
000662      905 FORMAT(//,8H LN(E)= ,1PE18.11,3X,1PE18.11,5HNLV ,1PE18.11,6HNLV*2
000662      1 ,1PE18.11,6HNLV*3 ,1PE18.11,5HNLV*4)
000662      906 FORMAT(//,36H THE CONSTANT ADDED TO ENERGIES WAS ,1PE18.11)
000662      907 FORMAT(//,126H PRESSURE (MBARS) VOLUME (CC/GM) TEMPER
000662      1ATURE (DEG K) ENERGY+C (MB-CC/GM) GAMMA (-DLNP/DLNV) PARTICLE
000662      2VELOCITY)
000662      908 FORMAT(6(3X,1PE18.11))
000662      909 FORMAT(70H1 THE ISENTROPE STATE VARIABLES AS COMPUTED FROM THE LEA
000662      1ST SQUARES FIT)
000662      910 FORMAT(//,119H BKW PRESSURE FIT PRESSURE BKW TE
000662      1MPERATURE FIT TEMPERATURE BKW ENERGY + C FIT ENER
000662      2Y)
000662      911 FORMAT (64H1 THE ISENTROPE PRESSURE AND COMPOSITION OF DETONATION
000662      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),
1FRENE(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,P0,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 TOF (TEMP,THERC(1,J),2,FRENE(J))
000121 FRENE(J)=FRENE(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,FRENE(J))
000165      FRENE(J)=(FRENE(J))/(R1)+(THERC(7,J)/R1)
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      FRENE(J)=FSP/R2T *FRENE(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,FRENE,ELEM,M,N,NT,IND)
000254      IF (IND.EQ.-1) GO TO 113
000256      IF (IND.EQ.-7) RETURN
000260      AMOLER=0.
000261      DO 114 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),
1FRENE(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,I0NL,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,ASROS(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      EGT=0.
000003      DO 201 I=1,N
000005      CALL TDF(TEMP,THERC(1,I),1,HHMO)
000012      EGT=EGT+(X(I)/XBAR)*(HHMO-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,HHMO)
000054      SESP(3) =VSOL(J)
000057      CALL SES(SESP,SOLEQS(1,J),2,ESP)
000064      ES(J)= HHMO *THERC(7,I) * (R3)*(ESP)

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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

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SUBROUTINE SYS2A (IND)
C  SYSTEM II A GIVEN P COMPUTE HUGONIOT TEMPERATURE
C  IND IS -1 FOR VGAS LFB 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),
1FRENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,E0,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),EXITIME,SESP(3),R1,R2,ABTOA
1,R3,R5,R6,SCALF,P0,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),VAMX(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 P0/.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-E0-(0.5)*(PRESS*P0)*(VO-VPG)*R3*AMOLWT)
000033  GO TO 249
000033 252 RETURN
000034  END

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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),
1FRENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,E0,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),EXITIME,SESP(3),R1,R2,ABTOA
1,R3,R5,R6,SCALF,P0,HUGBOS(10),CJBOS(4),APGCJ,BPGCJ
2,DELP,AMHUGP,HUGP(20),HUGT(20),HUGV(20),HUGUP(20),HUGUS(20)

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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,V0
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=(V0)*(SQRT((PRESS-P0)/( V0 -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*(V0-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),THERC(8,25),SOLEQS(12,5),AIK(250),VSOL(5),
1FRENE(25),XN1(25),ESOL(5),ELEM(10),N,NT,M,TEMP,PRESS,ALPHA,
2BETA,THETA,AKAPPA,VGAS,RHO,AMOLWT,E0,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,AHTOA
1,R3,R5,R6,SCALF,P0,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,V0
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

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```

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

```

```

C SUBROUTINE SYS4A (IND)
  SYSTEM 4A TO COMPUTE 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,E0,IOEQ,ICJC,IHUG,IPVC,
  3IGRP,IOIC,IRHO,IONL,IMIS,IEXT,FX,R1T,R2T,XBAR,
  4ETOT,VTOT,VP,ES(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
  5,VCJ,UCJ,CJT,CJS
000003 COMMON / RST/ VBOS(10),EXITIME,SESP(3),R1,R2,ABTOA
  1,R3,R5,R6,SCALF,P0,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),VROS2,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-E0)/(R3*AMOLWT) *CPRIME
000033 ASP(I)=PRESS
000035 ASV(I)=VP
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

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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* A1NCP
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

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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

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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,E0,IOEQ,ICJC,IHUG,IPVC,
3IGRP,IDIC,IRHO,I0NL,IMIS,IEXT,FX,HIT,R2T,XBAR,
4ETOT,VTOT,VPGE,ES(5),IND,GAMMA,DETVEL,PCJ,FGP,ALNP,S(25),SGAS,STOT
5VCJ,UCJ,CJT,CJS
000003      COMMON / RST/ VBOS(10),EXITME,SESP(3),R1,R2,ABTOA
1,R3,R5,R6,SCALF,P0,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-P0)/( 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

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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 8KW 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 8 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

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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
000260      C      PUT ANSWERS IN X
000262      DO 18 I=1,NTOT
000266      X(I)=BMAT(I)
000271      18 CONTINUE
000272      C      TEST FOR TOO SMALL X
000300      DO 19 I=1,NGAS
000303      IF (X(I).LT.AMINX) X(I)=AMINX
000304      19 CONTINUE
000307      C      TEST TO SEE IF ANY SOLIDS DISAPPEARED
000311      IF (NN1.EQ.0) GO TO 20
000312      I=NGAS+1
000315      DO 20 J=1,NN1
000316      IF (X(I).LT.0.) GO TO 50
000317      I=I+1
000325      20 CONTINUE
000327      C      TEST TO SEE IF CONVERGED
000331      SUM=0.
000333      DO 21 I=1,NTOT
000337      SUM=SUM+ABS(Y(I)-X(I))
000342      21 CONTINUE
000342      C      IF (SUM.LT.4MAXF) GO TO 60
000344      RESOLVE WITH Y NOW HAVING LAST ANSWERS X
000344      31 DO 32 I=1,NTOT
000344      Y(I)=X(I)
000347      32 CONTINUE
000347      GO TO 35
000347      C      HAVE CONVERGED
000347      60 DO 38 I=1,NTOT
000347      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
000363      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
000371      C      AN ERROR HAS OCCURRED AS OTHER THAN LAST SOLID DISAPPEARED
000373      C      IND=-1 IF ERROR HAS OCCURRED
000373      33 IND=-1
000373      RETURN
000373      C      ERROR HAS OCCURRED MATRIX IS SINGULAR
000375      40 IND=-7
000375      RETURN
000375      END

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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 SUCCEEDING 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

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000133 C SET COUNT NEGATIVE AND EXIT
000135 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) GO TO 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

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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 V0,A,B,C,D,E,A1,A2,C1,C2,C3,MOLWT
C IND= 0 FOR VOLUME, 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 RKW 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 LFR(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(1)=(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(1)=(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

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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

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      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=HO
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=HO/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

```

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      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)      A(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(IN)
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

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000053      X = ARS(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

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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

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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      R = COEFFICIENTS TO FIT
C      SB = ESTIMATE OF ERRORS IN COEFFICIENTS TO FIT
C      T = COEFFICIENTS TO ORTHOGONAL POLYNOMIALS
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=PXFP(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=XPXP
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

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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=1,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

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```

000005      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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