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SOLGASMIX-PV, a Computer Program to Calculate Equilibrium Relationships in Complex Chemical Systems

Theodore M. Besmann

MASTER

OAK RIDGE NATIONAL LABORATORY

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RELATIONSHIPS IN COMPLEX CHEMICAL SYSTEMS

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SOLGASMIX-PV, A COMPUTER PROGRAM TO CALCULATE EQUILIBRIUM
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Theodore M. Besmann

ABSTRACT

The use of the computer program SOLGASMIX-PV for calculating equilibrium compositions is described. The program can calculate equilibria in systems containing a gaseous phase, condensed phase solutions, and condensed phases of invariant or variable stoichiometry. Either a constant total gas volume or a constant total pressure can be assumed. Unit activities for condensed phases and ideality for solutions are assumed, although nonideal systems can be handled provided activity coefficient relationships are available.

INTRODUCTION

Chemical equilibrium calculations involve finding the system composition, within certain constraints, which contains the minimum free energy. The constraints are the preservation of the masses of each element present and either constant pressure or volume.

Numerous methods have been reported for computing thermodynamic equilibrium compositions. All the techniques, however, are based on the methods of either Brinkley^{1,2} or White et al.³ The method first outlined by Brinkley is the oldest and more indirect technique, requiring the determination of equilibrium constants. A simpler, more direct technique was first suggested by White et al. This method computes the equilibrium composition by the direct minimization of the system free energy. This eliminates the necessity of writing chemical equations and simplifies the addition or removal of species from the calculation. Eriksson⁴ has extended the technique to include systems containing multiple condensed phases and has developed a computer program, SOLGAS, for performing the calculations. Eriksson and Rosén⁵ have expanded the method to also handle liquid and solid, as well as

gaseous, mixtures (i.e., condensed phase solutions). Note that a mixture is defined as a combination of more than one species in a single phase. Eriksson⁶ has included this capability in a new program called SOLGASMIX which has the ability to calculate equilibria containing gases, condensed phases of invariant and variable stoichiometry, and mixtures at constant total pressure and temperature. Ideal gas phase and condensed phase solutions are assumed with unit activities for condensed phases, although nonideal systems can be handled provided activity coefficient relationships are available.

The author used the ideal gas law to slightly modify SOLGASMIX; hence, the program is now capable of calculating equilibria at a constant total gas volume with variable total pressure. The input scheme has also been modified so that it is easier to vary the input parameters. The new version is called SOLGASMIX-FV, and copies of the deck are available from the author.

In certain cases, the program will be unable to calculate an equilibrium composition. The statement "THE EQUILIBRIUM COMPOSITION HAS NOT BEEN OBTAINED" will be printed. This can only be overcome by changing some of the input parameters.

BASIC EQUATIONS

The total Gibbs free energy of a system can be expressed:

$$G_T = \sum_i n_i (G_i^O + RT \ln a_i) ,$$

where

G_T = total Gibbs free energy,

n_i = moles of species i ,

G_i^O = standard Gibbs free energy of species i ,

R = ideal gas law constant,

T = absolute temperature,

a_i = activity of species i .⁵

The total free energy can be conveniently written as the dimensionless quantity G_T/RT , and assuming ideality,

$$\begin{aligned}
\frac{G_T}{RT} = & \sum_{i=1}^{m_p} n_{pi} \left[\left(G^\circ/RT \right)_{pi} + \ln P + \ln \left(n_{pi}/N_p \right) \right]_{p=1} \\
& + \sum_{p=2}^{q+1} \sum_{i=1}^{m_p} n_{pi} \left[\left(G^\circ/RT \right)_{pi} + \ln \left(n_{pi}/N_p \right) \right] \\
& + \sum_{p=q+2}^{q+s+1} \sum_{i=1}^{m_p} n_{pi} \left(G^\circ/RT \right)_{pi} ,
\end{aligned}$$

where

m_p = number of species in phase p ,

P = total pressure,

N_p = moles of phase p .⁵

The phases are numbered consecutively from $p = 1$ for the gaseous phase, to $p = 2$ to $p = (q + 1)$ for condensed phase solutions, up to $p = (q + s + 1)$ for the last invariant condensed phase. In variable P and constant total gas volume (V) calculations, P is derived from:

$$P = \frac{N_1 RT}{V} .$$

The constraint that the masses of all elements must be conserved is provided by the subsidiary relationship:

$$\sum_{p=1}^{q+s+1} \sum_{i=1}^{m_p} A_{pij} n_{pi} = b_j ,$$

where

A_{pij} = coefficient on element j of species i in phase p ,

b_j = g-atoms of element j .⁵

The minimum total Gibbs free energy is calculated by solving the above set of equations using Lagrange's method of undetermined multipliers and Taylor expansions about an arbitrary point (the moles of each species), neglecting terms involving derivatives of second and higher orders. The activity coefficient, γ_{pi} , from the relationship

$$a_{pi} = \gamma_{pi} (n_{pi}/N_p)$$

can be introduced in the calculations for the purpose of including deviations from ideality.

OPERATIONAL FEATURES

The program is designed to handle a maximum of 10 elements, 99 substances, and 10 mixtures, where the gas phase is considered a mixture. Each substance is either a gas or condensed phase species, or a member of a condensed phase mixture.

The relationships giving the nonunit activity coefficients and describing variable stoichiometries are written by the user and appear in the subroutine FACTOR. The quantities that can be used in the relationships are:

AO (I,J) = a variable stoichiometric coefficient, where I is the species number and J is the element number,

AKT (I) = activity,

AKTF (I) = activity coefficient,

Y (I) = amount (mole) of species,

YF (I) = mole fraction or partial pressure.

A subroutine named SPEQUA is provided for calculating quantities which can be derived from the equilibrium composition. The user writes the equations for any parameters of interest, using the values generated by the program, and inserts them in SPEQUA along with an appropriate output format. In order to speed the calculations, any substance computed to be $< 1 \times 10^{-20}$ mole is set equal to zero. This fact must be considered when using the program and particularly when using the subroutine FACTOR.

Complex multiphase systems have been run on an IBM 360/91 using <256 K of core and <30 sec.

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APPENDIX A. INPUT DATA GUIDE FOR SOLGASMIX-PV

<u>Card</u>	<u>Columns</u>	<u>Variable name</u>	
1	1-80	TITLE	Anything punched on this card will be repeated at the top of every page of output.
2	1-2	L	The number of elements in the system considered (≤ 10).
	3-4	MP	The total number of gaseous, liquid, and solid mixtures (≤ 10).
	5-6	MR	The total number of condensed phases of invariant stoichiometry.
	7-8	ML	The total number of species in mixture No. 1 (the gas phase).
	9-10		The total number of species in mixture No. 2, etc. Format is (40I2).
3	1-8	EL	Symbol for element No. 1.
	9-16		Symbol for element No. 2, etc. Note: the symbols are left adjusted. Format is (10A8).
4	1-5	A	The coefficient on the elemental symbol of element No. 1 in species No. 1.
	6-10		The coefficient on the elemental symbol of element No. 2 in species No. 1, etc. Format is (16F5.0). Note: there is one card per species. The species must appear such that the gases are first followed by the mixtures in the same order as card No. 2, and the invariant condensed phases follow last. A compound can be considered an element provided its activity can be specified.
5	1	NV	= 0 if the calculations are to be performed at constant pressure; continue with card No. 6. = 1 if the calculations are to be performed at constant volume.
	11-20	V	System volume in liters. Format is (11,9X, E10.0).

<u>Card</u>	<u>Columns</u>	<u>Variable name</u>	
6	1-2	IEL	The species number, from the order of the substances in card No. 4, for element No. 1 in its chosen reference state.
	3-4		The species number, from the order of the substances in card No. 4, for element No. 2 in its chosen reference state, etc. Format is (40I2).
7	2	MGT	The maximum number of coefficients in the expression $\Delta G^{\circ} \text{ (J}\cdot\text{mole}^{-1}) = a/T + b + cT + dT^2 + eT^3 + fT \ln T$, which can be different from zero for the species considered to be present.
	3-4	MOK	The number of species with values of $(G^{\circ} - H_{298}^{\circ})/T$ or ΔH_{298}° unknown. Note: MGT = 0 and MOK = 0 if values of $(G^{\circ} - H_{298}^{\circ})/T$ and ΔG° are used as input data, respectively. Format is (40I2). Continue with card Nos. 10, 11, 12, and 15 if MGT > 0. Continue with card Nos. 9, 12, 13, and 15 if MGT and MOK = 0. Continue with card Nos. 8, 9, 12, 13, and 15 if MOK > 0.
8	1-2	IOK	The number for one of the species with values of $(G^{\circ} - H_{298}^{\circ})/T$ or ΔH_{298}° unknown.
	3-4		The number for another of these species, etc. Format is (40I2).
9	1-8	TEXT	Name of species No. 1.
	11-20	HF	ΔH_{298}° (kJ·mole ⁻¹) for the formation of species No. 1, etc., with one card per species appearing in the same order as in card No. 4.
10	2	IGT	The number for one of the nonzero coefficients in the expression for ΔG° .
	4		The number for another of the nonzero coefficients, etc. Coefficient No. 1 is a, No. 2 is b, etc. Format is (40I2).

<u>Card</u>	<u>Columns</u>	<u>Variable name</u>	
11	1-8	TEXT	Name of species No. 1.
	11-20	GE	The value of coefficient No. IGT(1) for species No. 1.
	21-30		The value of coefficient No. IGT(2) for species No. 1, etc. There is one card for each species in the same order as the species appear in card No. 4. Format is (A8,2X,7E10.3).
12	1-10	T	The reaction temperature (K). Format is (E10.0).
13	1-10	FEF	$(G^\circ - H_{298}^\circ)/T$ ($J \cdot K^{-1} \text{ mole}^{-1}$) for species No. 1, etc., with one card per species appearing in the same order as in card No. 4.
14	1-10	PTOT	The total pressure (atm). Format is (E10.0).
15	2	KVALL	<p>= 1 if a starting estimate will be supplied manually; continue with card Nos. 16, 17, 18, 19, and 15.</p> <p>= 2 if a starting estimate generated by the program will be used; continue with card Nos. 16, 17, 18, and 15.</p> <p>= 3 if the values of NPKT, KH, and B (cf. card Nos. 16, 17, and 18) to be used in the next group are different from the values used in the preceding group; continue with card Nos. 16, 17, 18, and 15.</p> <p>= 4 if the values of NPKT and KH to be used in the next group are equal to the values used in the preceding group whereas the values of B are different; continue with card Nos. 18 and 15.</p> <p>= 5 if the values of NPKT, KH, and B to be used in the next group are equal to the values used in the preceding group; continue with card No. 15.</p> <p>= 6 at a transfer to a new value of the temperature. Continue with card Nos. 12 and 15 if MGT > 0 and with card Nos. 12, 13, and 15 if MGT and MOK = 0 or if MOK > 0.</p>

<u>Card</u>	<u>Columns</u>	<u>Variable name</u>	
15 (cont.)			<p>= 7 if NV = 0 and the total pressure is different from 1 atm or at a transfer to a new value of the total pressure; continue with card No. 14.</p> <p>= 8 at a transfer to new expressions for ΔG^0; continue with card Nos. 10, 11, and 15.</p> <p>= 9 at a transfer to a new system; continue with card No. 1.</p>
	1-2		= 10 if the calculations are ended. Format is (I2).
16	1-2	NPKT	The number of calculations to be performed using different total amounts of each element or different activities of each element (≤ 99). Format is (I2).
17	2	KH	The variation of the total amount or of the known equilibrium activity (a) for element No. 1.
	4		<p>The variation of the total amount or of the known equilibrium activity for element No. 2, etc. Format is (40I2).</p> <p>Note: KH = 1 The total amount varies irregularly.</p> <p>KH = 2 The total amount is constant.</p> <p>KH = 3 The total amount varies by a constant increment.</p> <p>KH = 4 Log (a) varies irregularly.</p> <p>KH = 5 Log (a) is constant.</p> <p>KH = 6 Log (a) varies by a constant increment.</p>
18a	1-10	B	The total amount (g-atom) for one element or log (a) for the element in its chosen reference state for the first calculation.
	11-20		The total amount (g-atom) or log (a) for the second calculation, etc. If all 80 columns are filled, start a new card.
18b	1-10	B	The total amount (g-atom) or log (a).
18c	1-10	B	The initial total amount (g-atom) or log (a) for one element.

<u>Card</u>	<u>Columns</u>	<u>Variable name</u>	
18c (cont.)	11-20	STEP	The increment in the total amount (g-atom) or log (a).
			One card is punched for each element in the order they appear in card No. 3. Card No. 18a is used if KH = 1 or 4, card No. 18b is used if KH = 2 or 5, and card No. 18c is used if KH = 3 or 6. Format is (8E10.0).
19	1-10	Y	Initial estimate (mole) for each species with one card per species appearing in the same order as in card No. 4. Format is (E10.0).

APPENDIX B. EXAMPLE OF INPUT AND OUTPUT

For illustrative purposes, the chemical system containing plutonium, carbon, and oxygen in the presence of argon was input to SOLGASMIX-PV, and equilibrium compositions were computed. Argon is added to maintain the constant pressure indicated. The system is assumed to contain two mixtures, a gas phase consisting of Ar, CO, CO₂, O₂, Pu, PuO, PuO₂, and PuC₂, and an ideal solid solution composed of PuO_(s) and PuC_(s). There are also a number of invariant condensed phases to be considered: C, Pu_(l), Pu₂O₃, Pu₂C₃, and PuC.

The calculations are to be performed for a constant pressure system (1.0 atm). The thermodynamic data are in the form:

$$\Delta G^{\circ} \text{ (J.mole}^{-1}\text{)} = b + cT,$$

and therefore free energy functions (fef) and ΔH_{298}° values are not used. The absolute temperature is 1900 K.

In this example, starting estimates of the equilibrium moles of each species are generated by the program. Two series of calculations are called for. The first uses 0.1 g-atom argon, 1.0 g-atom plutonium, 1.0 g-atom carbon, and 0.1 g-atom oxygen. The second is conducted using 0.1 g-atom less carbon and 0.05 g-atom more oxygen.

1
2
3
4

01	02	03	04	05	06	07	08	09	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640	641	642	643	644	645	646	647	648	649	650	651	652	653	654	655	656	657	658	659	660	661	662	663	664	665	666	667	668	669	670	671	672	673	674	675	676	677	678	679	680	681	682	683	684	685	686	687	688	689	690	691	692	693	694	695	696	697	698	699	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764	765	766	767	768	769	770	771	772	773	774	775	776	777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000
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Card
No.

[illegible]

PU - C - O TEST

NO. OF ELEMENTS = 4 NO. OF MIXTURES = 2 NO. OF INVARIANT SOLIDS = 5

NC. OF SPECIES PER MIXTURE = 8, 2,

SPECIES	A	B	C	D	E	F
AR	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	-0.11729D 06	-0.84390D 02	0.0	0.0	0.0
CO2	0.0	-0.39622D 06	-0.13000D 00	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0
PU	0.0	0.32680D 06	-0.88830D 02	0.0	0.0	0.0
PUO	0.0	-0.11900D 06	-0.41000D 02	0.0	0.0	0.0
PUO2	0.0	-0.47110D 06	0.28000D 02	0.0	0.0	0.0
PUC2	0.0	0.15690D 06	-0.21000D 02	0.0	0.0	0.0
PUO (S)	0.0	-0.55733D 06	0.92300D 02	0.0	0.0	0.0
PUC (S)	0.0	-0.32500D 05	-0.12300D 02	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0
PU	0.0	0.0	0.0	0.0	0.0	0.0
PU2O3	0.0	-0.16720D 07	0.26700D 03	0.0	0.0	0.0
PU2C3	0.0	-0.16400D 06	0.78400D 01	0.0	0.0	0.0
PUC	0.0	-0.32500D 05	-0.12300D 02	0.0	0.0	0.0

PU - C - O TEST

SUBSCRIPTS ON ELEMENTAL SYMBOLS OF EACH SPECIES

	AR	PU	C	O
AR	1.00	0.0	0.0	0.0
CO	0.0	0.0	1.00	1.00
CO2	0.0	0.0	1.00	2.00
O2	0.0	0.0	0.0	2.00
PU	0.0	1.00	0.0	0.0
PUO	0.0	1.00	0.0	1.00
PUO2	0.0	1.00	0.0	2.00
PUC2	0.0	1.00	2.00	0.0
PUO(S)	0.0	1.00	0.0	1.00
PUC(S)	0.0	1.00	1.00	0.0
C	0.0	0.0	1.00	0.0
PU	0.0	1.00	0.0	0.0
PU2O3	0.0	2.00	0.0	3.00
PU2C3	0.0	2.00	3.00	0.0
PUC	0.0	1.00	1.00	0.0

T = 1900.00 K

PU - C - O TEST

T = 1900.00 K
P = 1.000D 00 ATM

	X*/MOLE	Y/MOLE	P/ATM	ACTIVITY
AR	0.10000D 00	0.10000D 00	0.99989D 00	0.99989D 00
CO	0.0	0.10004D-04	0.10003D-03	0.10003D-03
CO2	0.0	0.35154D-12	0.35150D-11	0.35150D-11
O2	0.50000D-01	0.36109D-22	0.36105D-21	0.36105D-21
PU	0.0	0.93972D-06	0.93961D-05	0.93961D-05
PUO	0.0	0.10215D-06	0.10214D-05	0.10214D-05
PUO2	0.0	0.23106D-11	0.23104D-10	0.23104D-10
PUC2	0.0	0.18981D-06	0.18979D-05	0.18979D-05
			MOLE FRACTION	
PUO (S)	0.0	0.99990D-01	0.12498D 00	0.12498D 00
PUC (S)	0.0	0.70005D 00	0.87502D 00	0.87502D 00
C	0.10000D 01	0.0		
PU	0.10000D 01	0.0		
PU2O3	0.0	0.0		
PU2C3	0.0	0.99981D-01		
PUC	0.0	0.0		

PU - C - O TEST

T = 1900.00 K
P = 1.000D 00 ATM

	X*/MOLE	Y/MOLE	P/ATM	ACTIVITY
AR	0.10000D 00	0.10000D 00	0.99982D 00	0.99982D 00
CO	0.0	0.17023D-04	0.17020D-03	0.17020D-03
CO2	0.0	0.92322D-12	0.92305D-11	0.92305D-11
O2	0.75000D-01	0.86016D-22	0.86001D-21	0.86001D-21
PU	0.0	0.81186D-06	0.81171D-05	0.81171D-05
PUO	0.0	0.13621D-06	0.13619D-05	0.13619D-05
PUO2	0.0	0.47550D-11	0.47542D-10	0.47542D-10
PUC2	0.0	0.19931D-06	0.19927D-05	0.19927D-05
			MOLE FRACTION	
PUO(S)	0.0	0.14998D 00	0.16664D 00	0.16664D 00
PUC(S)	0.0	0.75008D 00	0.83336D 00	0.83336D 00
C	0.90000D 00	0.0		
PU	0.10000D 01	0.0		
PU2O3	0.0	0.0		
PU2C3	0.0	0.49967D-01		
PUC	0.0	0.0		

IHC002I STOP 00000

APPENDIX C. SOLGASMIX-PV LISTING

THEODORE M. BESMANN

OAK RIDGE NATIONAL LABORATORY
OAK RIDGE, TN 37830

CALCULATES EQUILIBRIA AT CONSTANT PRESSURE OR VOLUME. THE PROGRAM IS A MODIFICATION OF SOLGASMIX (G. ERIKSSON, CHEMICA SCRIPTA., 8 (1975) 100).

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IMPLICIT REAL*8 (A-H,O-Z)
COMMON A(99,10), AO(99,10), AKT(99), AKTF(99), B(10,99), BO(10),
$G(99), KH(20), L, M, M1, MA, MB, MF(20), ML(20), MP, MS, NO(99),
$NP, PI(20), PTOT, T, TEXT(99), Y(99), YF(99), YTOT(20), V, NV, NVV
DIMENSION PEF(99), GE(99,6), HF(99), IEL(10), IFM(15), IGT(6),
$IOK(99), XI(99), TITLE(10), EL(10), GY(99,6)
H = DLOG(10.)
IN=5
IOUT=6
MP(1) = 1
26 PTOT = 1.
DO 48 K = 1, 20
48 KH(K) = 0
READ (IN,240) (TITLE(I), I=1,10)
240 FORMAT (10A8)
WRITE (IOUT,230) (TITLE(I), I=1,10)
230 FORMAT ('1',20X,10A8)
READ (IN,102) L, MP, MR, (ML(M), M = 1, MP)
102 FORMAT (40I2)
WRITE (IOUT,250) L, MP, MR, (ML(M), M=1, MP)
250 FORMAT ('0NO. OF ELEMENTS = ',I2,5X,'NO. OF MIXTURES = ',I2,5X,
1'NO. OF INVARIANT SOLIDS = ',I2/, '0NO. OF SPECIES PER MIXTURE = ',
210(I2,', '))
IF (MP .EQ. 1) GO TO 146
DO 132 M = 2, MP
MF(M) = ML(M-1) + 1
132 ML(M) = ML(M-1) + ML(M)
146 M1 = ML(MP) + 1
MS = ML(MP) + MR
READ (IN,260) (EL(I), I=1,L)
260 FORMAT (10A8)
DO 33 I = 1, MS
XI(I) = 0.
READ (IN,280) (A(I,J), J=1,L)
280 FORMAT (16F5.0)
DO 33 J = 1, L
33 AO(I,J) = A(I,J)
READ (IN,200) NV,V
200 FORMAT (I1,9X,E10.0)
READ (IN,102) (IEL(J), J = 1, L)
READ (IN,102) MGT, MOK
IF (MGT .GT. 0) GO TO 14

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      IF (MOK .GT. 0) READ (IN,102) (IOK(N), N = 1, MOK)
      DO 255 I=1,MS
255 READ (IN,270) TEXT(I),HF(I)
270 FORMAT (A8,2X,7E10.3)
      GO TO 310
      14 READ (IN,102) (IGT(N), N = 1, MGT)
      85 DO 265 I=1,MS
265 READ (IN,270) TEXT(I), (GE(I,N), N=1,MGT)
      DO 266 I=1,MS
      DO 267 N=1,6
267 GY(I,N)=0.
      DO 266 N=1,MGT
266 GY(I,IGT(N))=GE(I,N)
      WRITE (IOUT,300) (TEXT(I), (GY(I,N), N=1,6 ), I=1,MS)
300 FORMAT ('0SPECIES',6X,'A',14X,'B',14X,'C',14X,'D',14X,'E',14X,'F',
1/,99('0',A8,3X,6(E12.5,3X),/))
310 WRITE (IOUT,230) (TITLE(I), I=1,10)
      WRITE (IOUT,340) (EL(I), I=1,L)
340 FORMAT ('0',20X,'SUBSCRIPTS ON ELEMENTAL SYMBOLS OF EACH SPECIES',
1/, '0',18X,10(A8,2X))
      DO 350 I=1,MS
350 WRITE (IOUT,360) TEXT(I), (A(I,J), J=1,L)
360 FORMAT ('0',A8,8X,10(F5.2,5X))
      42 READ (IN,103) T
      WRITE (IOUT,122) T
122 FORMAT (4H0T =, F8.2, 2H K/)
      IF (MGT .EQ. 0) GO TO 82
      DO 84 I = 1, MS
84 G(I) = 0.
      DO 81 N = 1, MGT
      IF (IGT(N) .LT. 6) TP = T** (IGT(N) - 3)/8.31433
      IF (IGT(N) .EQ. 6) TP = DLOG(T)/8.31433
      DO 81 I = 1, MS
81 G(I) = G(I) + GE(I,N)*TP
      GO TO 8
82 DO 49 I = 1, MS
      READ (IN,103) FEF(I)
49 G(I) = (FEF(I) + 1000.*HF(I)/T)/8.31433
      IF (MOK .EQ. 0) GO TO 4
      DO 23 N = 1, MOK
      I = IOK(N)
      G(I) = -H*FEF(I)
      DO 23 J = 1, L
      K = IEL(J)
23 G(I) = G(I) + A(I,J)/A(K,J)*G(K)
      4 WRITE (IOUT,230) (TITLE(I), I=1,10)
      WRITE (IOUT,106) (TEXT(I), HF(I), FEF(I), G(I), I = 1, MS)
106 FORMAT (15X, 5HHF298, 8X, 3HFEF, 9X, 4HG/RT/(' ',A8,F12.0,2F12.3))
      GO TO 8
37 READ (IN,103) PTOT
103 FORMAT (8E10.0)
      8 READ (IN,102) KVAL1
      GO TO (40,40,40,7,34,42,37,85,26,1), KVAL1
40 READ (IN,102) NPKT
      READ (IN,102) (KH(J), J = 1, L)
      7 DO 164 J = 1, L
      N = KH(J)

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      GO TO (161,162,163,161,162,163), N
161 READ (IN,103) (B(J,N), N = 1, NPKT)
      GO TO 164
162 READ (IN,103) B(J,1)
      IF (NPKT .EQ. 1) GO TO 164
      DO 160 N = 2, NPKT
160 B(J,N) = B(J,1)
      GO TO 164
163 READ (IN,103) B(J,1), STEP
      DO 165 N = 2, NPKT
165 B(J,N) = B(J,N-1) + STEP
164 CONTINUE
      GO TO (35,39,34,34), KVAL1
      35 DO 370 I=1,MS
370 READ (IN,103) Y(I)
      GO TO 166
      39 BEST = 0.
      DO 169 J = 1, L
      IF (B(J,1) .GT. BEST .AND. KH(J) .LT. 4) BEST = B(J,1)
169 CONTINUE
      BEST = BEST/DFLOAT(MS)
      DO 167 I = 1, MS
167 Y(I) = BEST
166 DO 135 M = 1, MP
      YTOT(M) = 0.
      MA = MF(M)
      MB = ML(M)
      DO 135 I = MA, MB
135 YTOT(M) = YTCT(M) + Y(I)
      34 NP = 0
      27 NP = NP + 1
      DO 75 I = 1, MS
      75 NO(I) = 1
      DO 22 J = 1, L
      B0(J) = B(J,NP)
      I = IEL(J)
      IF (KH(J) .LT. 4) GO TO 170
      PI(J) = (G(I) + H*B0(J))/A(I,J)
      GO TO 22
170 XI(I) = B0(J)/A(I,J)
      IF (EO(J) .NE. 0.) GO TO 22
      DO 30 I = 1, MS
      IF (A(I,J) .EQ. 0.) GO TO 30
      NO(I) = 0
      Y(I) = 0.
      30 CONTINUE
      22 CONTINUE
      CALL GASOL
      WRITE (IOUT,230) (TITLE(I), I=1,10)
      WRITE (IOUT,111) T, PTOT
111 FORMAT (4H0T =, F8.2, 2H K/ 4H P =, 1PE10.3, 4H ATM/)
      IF (NV.EQ.0) GO TO 210
      WRITE (IOUT,220) V
220 FORMAT (4H V =, 1PE10.3, 2H L/)
210 CONTINUE
      IF (M .LE. MP) GO TO 64
      WRITE (IOUT,118)

```

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118 FORMAT (/50H THE EQUILIBRIUM COMPOSITION HAS NOT BEEN OBTAINED)
      GO TO 28
      64 IF (M .EQ. 0) WRITE (IOUT,121)
121 FORMAT (33H THE SMALL Y-VALUES ARE NOT EXACT/)
      DO 17 J = 1, L
      IF (KH(J) .LT. 4) GO TO 17
      K = IEL(J)
      XI(K) = 0.
      DO 50 I = 1, MS
      50 XI(K) = XI(K) + A0(I,J)*Y(I)
      17 CONTINUE
      WRITE (IOUT,105)
105 FORMAT (15X,7HX*/MOLE,8X,6HY/MOLE,10X,5HP/ATM,8X,8HACTIVITY)
      DO 140 M = 1, MP
      IF (M .GT. 1) WRITE (IOUT,125)
125 FORMAT (41X, 13HMOLE FRACTION)
      MA = MF(M)
      MB = ML(M)
      DO 140 I = MA, MB
140 WRITE (IOUT,124) TEXT(I), XI(I), Y(I), YF(I), AKT(I)
124 FORMAT (' ',A8,4(3X,E12.5))
      IF (MR .GT. 0) WRITE (IOUT,120) (TEXT(I), XI(I), Y(I), I = M1, MS)
120 FORMAT (/(' ',A8,2(3X,E12.5)))
      CALL SPEQUA
      28 IF (NP - NPKT) 27,8,8
      1 STOP
      END

```

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SUBROUTINE GASOL
  IMPLICIT REAL*8 (A-H,O-Z)
  COMMON A(99,10), AO(99,10), AKT(99), AKTF(99), B(10,99), BO(10),
  $G(99), KH(20), L, M, M1, MA, MB, MF(20), ML(20), MP, MS, NO(99),
  $NP, PI(20), PTOT, T, TEXT(99), Y(99), YF(99), YTOT(20), V, NV, NVV
  DIMENSION F(99), IFAS(20), ISOL(20), LX(99), NSUM(500), OPI(10),
  $R(20,21), YFTOT(20), YX(99)
  MX = 0
171 IS = -1
  MSUM = 0
  NG = 0
55 ISUM = 0
  MSA = 0
  IF (MS .LT. M1) GO TO 47
  DO 52 I = M1, MS
  IF (Y(I) .EQ. 0.) GO TO 52
  MSA = MSA + 1
  ISOL(MSA) = I
  ISUM = ISUM + 2**(I + MP - M1)
52 CONTINUE
47 MPA = 0
  NG = NG + 1
  IF (NG .EQ. 501) NG = 1
  NSUM(NG) = ISUM
  YSUM = 0.
  DO 152 M = 1, MP
  IF (YTOT(M) .EQ. 0.) GO TO 152
  MPA = MPA + 1
  IFAS(MPA) = M
  NSUM(NG) = NSUM(NG) + 2**(M - 1)
  YSUM = YSUM + YTOT(M)
152 CONTINUE
  IF (NSUM(NG) .GE. IS .AND. MPA + MSA .LE. L) GO TO 69
59 IS = IS + 2
  DO 154 N = 1, MPA
  M = IFAS(N)
154 YTOT(M) = 0.
  ISUM = 0
  MPA = 1
  YTOT(1) = 1.
  IF (MSA .EQ. 0) GO TO 73
  DO 68 N = 1, MSA
  I = ISOL(N)
68 Y(I) = 0.
  MSA = 0
73 IF (IS .EQ. 1) GO TO 74
  IT = IS
61 M = 0
71 M = M + 1
  IF (2**M .LE. IT) GO TO 71
  IF (M .GT. MP) GO TO 57
  MPA = MPA + 1
  IFAS(MPA) = M
  YTOT(M) = 1.
  MA = MP(M)

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      MB = ML(M)
      DO 150 I = MA, MB
      IF (NO(I) .EQ. 1) Y(I) = YSUM
150 CONTINUE
      GO TO 136
57  I = M + ML(MF) - MP
      IF (I .GT. MS) RETURN
      IF (NO(I) .EQ. 0) GO TO 59
      MSA = MSA + 1
      ISOL(MSA) = I
      ISUM = ISUM + 2**(M - 1)
      Y(I) = YSUM
136 IT = IT - 2**(M - 1)
      IF (IT .GT. 1) GO TO 61
      IF (MPA + MSA .GT. L) GO TO 59
74  IFAS(1) = 1
      IF (NSUM(NG) .GT. IS) NG = NG + 1
      IF (NG.EQ.501) NG=1
      NSUM(NG) = IS
69  IF (NG .EQ. 1) GO TO 129
      DO 148 K = 2, NG
      IF (NSUM(NG) .EQ. NSUM(K-1)) GO TO 59
148 CONTINUE
      IF (NSUM(NG-1) .EQ. MSUM) NSUM(NG-1) = -NSUM(NG-1)
      IF (NG.LT.3.OR.NSUM(NG-2).NE.-MSUM.OR.NSUM(NG).EQ.MSUM) GO TO 129
      NSUM(NG-2) = -NSUM(NG-2)
129 DO 142 M = 1, MP
      MA = MF(M)
      MB = ML(M)
      IF (YTOT(M) .GT. 0.) GO TO 130
      DO 126 I = MA, MB
      AKT(I) = 0.
      AKTF(I) = 1.
      Y(I) = 0.
126 YF(I) = 0.
      GO TO 142
130 DO 45 I = MA, MB
      IF (NO(I) .EQ. 1 .AND. Y(I) .LT. 1.E-8) Y(I) = 1.E-8
      AKTF(I) = 1.
45  LX(I) = 0
      CALL ABER
      IF (YTOT(M) .EQ. 0.) GO TO 47
142 CONTINUE
      LS1 = L + MPA + MSA
      LS = LS1 - 1
      LS2 = LS + 2
134 DMIN = 1.E-6
      IVAR = 0
      IVARJ = ML(1) - MS
16  DO 6 J = 1, LS1
      DO 6 K = J, LS2
6   R(J,K) = 0.
      DO 9 N = 1, MPA
      L1 = L + N
      M = IFAS(N)
      MA = MF(M)
      MB = ML(M)

```

```

DO 5 I = MA, MB
IF (Y(I) .EQ. 0.) GO TO 5
F(I) = G(I) + DLOG(AKT(I))
R(L1,LS2) = R(L1,LS2) + F(I)*Y(I)
DO 77 J = 1, L
IF (A(I,J) .EQ. 0.) GO TO 77
AY = A(I,J)*Y(I)
R(J,L1) = R(J,L1) + AY
R(J,LS2) = R(J,LS2) + AY*F(I)
DO 80 K = J, L
80 R(J,K) = R(J,K) + AY*A(I,K)
77 CONTINUE
5 CONTINUE
DO 9 J = 1, L
9 R(J,LS2) = R(J,LS2) - R(J,L1)
IF (MSA .EQ. 0) GO TO 63
DO 67 N = 1, MSA
I = ISOL(N)
K = L + MPA + N
R(K,LS2) = G(I)
DO 67 J = 1, L
67 R(J,K) = A(I,J)
63 DO 31 J = 2, LS1
N = J - 1
DO 31 K = 1, N
31 R(J,K) = R(K,J)
IF (MX .EQ. 0) GO TO 156
DO 131 J = 1, L
131 B0(J) = B(J,MP)
DO 172 N = 1, MPA
N = IFAS(N)
IF (MF(N) .NE. ML(N)) GO TO 172
MA = MF(N)
DO 89 J = 1, L
IF (A(MA,J) .EQ. A0(MA,J)) GO TO 89
AKVOT = (1. - A(MA,J)/A0(MA,J))*Y(MA)
DO 91 K = 1, L
IF (A(MA,K) .EQ. A0(MA,K)) B0(K) = B0(K) + AKVOT*A(MA,K)
91 CONTINUE
GO TO 172
89 CONTINUE
172 CONTINUE
156 DO 44 K = 1, L
IF (KH(K) .LT. 4) GO TO 44
DO 83 J = 1, LS1
83 R(J,LS2) = R(J,LS2) - PI(K)*R(J,K)
44 R(K,LS2) = R(K,LS2) + B0(K)
DO 10 K = 1, LS
IF (KH(K) .GT. 3) GO TO 10
ELMAX = 0.
DO 11 J = K, LS1
IF (ABS(R(J,K)) .LE. ELMAX .OR. KH(J) .GT. 3) GO TO 11
MROW = J
ELMAX = DABS(R(J,K))
11 CONTINUE
IF (ELMAX .GT. 0.) GO TO 36
IF (K .GT. L .OR. B0(K) .EQ. 0.) GO TO 10

```

```

GO TO 59
36 IF (MROW .EQ. K) GO TO 13
DO 15 N = K, LS2
RADBYT = R(MROW,N)
R(MRCW,N) = R(K,N)
15 R(K,N) = RADBYT
13 KA = K + 1
DO 46 J = KA, LS1
RKVOT = R(J,K)/R(K,K)
DO 46 N = KA, LS2
46 R(J,N) = R(J,N) - RKVOT*R(K,N)
10 CONTINUE
DO 20 N = 1, LS1
K = LS2 - N
IF (KH(K) .GT. 3) GO TO 20
IF (R(K,K) .NE. 0. .AND. R(K,LS2) .NE. 0.) GO TO 62
PI(K) = 0.
K = K - L - MPA
IF (K .LE. 0) GO TO 20
I = ISOL(K)
Y(I) = 0.
GO TO 55
62 PI(K) = R(K,LS2)/R(K,K)
KA = K - 1
IF (KA .EQ. 0) GO TO 20
DO 58 J = 1, KA
58 R(J,LS2) = R(J,LS2) - PI(K)*R(J,K)
20 CONTINUE
IF (IVAR .EQ. 0 .OR. IVARJ .GE. 0 .OR. SLAM .LT. 0.1) GO TO 66
DO 70 J = 1, L
IF (DABS(PI(J)) .GT. 1.E-8 .AND. DABS(OPI(J)/PI(J)-1.) .GT. DMIN)
1GO TO 65
70 CONTINUE
NR = 0
IF (NG .EQ. 1) GO TO 155
DO 157 K = 2, NG
IF (NSUM(NG) .EQ. -NSUM(K-1)) NR = NR + 1
157 CONTINUE
155 DO 143 M = 1, MP
IF (YTOT(M) .GT. 0.) GO TO 143
CALL XBER
YFTOT(M) = 0.
DO 144 I = MA, MB
YFTOT(M) = YFTOT(M) + YF(I)
YX(I) = YF(I)
AKT(I) = 0.
144 YF(I) = 0.
IF (NV.EQ.0) GO TO 326
YA=0.
DO 325 I=1,ML(1)
325 YA=Y(I)+YA
PTOT=YA*.0821*T/V
326 CONTINUE
IF (M .EQ. 1) YFTOT(M) = YFTOT(M)/PTOT
143 CONTINUE
145 DIFM = 1.
DO 158 M = 1, MP

```



```

      IF (YTOT(M) .GT. 0. .OR. YPTOT(M) .LE. DIFM) GO TO 158
      KA = M
      DIFM = YPTOT(M)
158  CONTINUE
      IF (DIFM .EQ. 1.) GO TO 138
      IF (NR .EQ. 0) GO TO 159
      NR = NR - 1
      YPTOT(KA) = 1.
      GO TO 145
159  MSUM = NSUM(NG)
      YTOT(KA) = 1.
      MA = MF(KA)
      MB = ML(KA)
      DO 153 I = MA, MB
153  Y(I) = YSUM*YX(I)/YPTOT(KA)
      GO TO 47
138  IF (MS .LT. M1) GO TO 51
      DIFM = 0.
      DO 54 I = M1, MS
      IF (NO(I) .EQ. 0 .OR. Y(I) .GT. 0.) GO TO 54
      PIA = -G(I)
      DO 56 J = 1, L
56  PIA = PIA + A(I,J)*PI(J)
      IF (PIA .LT. DIFM) GO TO 54
      KA = I
      DIFM = PIA
54  CONTINUE
      IF (DIFM .EQ. 0.) GO TO 51
      Y(KA) = YSUM
      GO TO 55
51  IF (MX .EQ. 1) GO TO 93
      DO 168 N = 1, MPA
      M = IFAS(N)
      IF (MF(M) .NE. ML(M)) GO TO 168
      MA = MF(M)
      DO 173 J = 1, L
      IF (A(MA,J) .EQ. A0(MA,J)) GO TO 173
      MX = 1
      GO TO 171
173  CONTINUE
168  CONTINUE
93  IVARJ = 0
      GO TO 66
65  DO 60 J = 1, L
60  OPI(J) = PI(J)
66  SLAM = 1.
      DO 12 N = 1, MPA
      L1 = L + N
      M = IFAS(N)
      MA = MF(M)
      MB = ML(M)
      DO 12 I = MA, MB
      IF (Y(I) .EQ. 0.) GO TO 12
      PIA = F(I) - PI(L1)
      DO 19 J = 1, L
19  PIA = PIA - A(I,J)*PI(J)
      YX(I) = PIA*Y(I)

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```

      IF (PIA .GT. SLAM) SLAM = PIA
12  CONTINUE
      IF (SLAM .GT. 1.) SLAM = 0.999*(SLAM - 0.5)/(SLAM*SLAM)
      IF (MSA .EQ. 0) GO TO 72
      DO 53 N = 1, MSA
        I = ISOL(N)
        K = I + MPA + N
        IF (PI(K) .LT. 0.) L1 = 0
        IF (IVAR .EQ. 0 .OR. PI(K) .GT. -Y(I)) GO TO 53
        IF (SLAM .LT. 1. .AND. -PI(K)/YSUM .LT. 1.E8) GO TO 53
        Y(I) = 0.
        GO TO 55
53  Y(I) = DABS(PI(K))
72  YSUM = 0.
      DO 128 N = 1, MPA
        M = IFAS(N)
        MA = MF(M)
        MB = ML(M)
        DO 29 I = MA, MB
          IF (Y(I) .EQ. 0.) GO TO 29
          Y(I) = Y(I) - SLAM*YX(I)
          IF (Y(I) .LT. 1.E-20) Y(I) = 0.
29  CONTINUE
      CALL ABER
      IF (YTOT(M) .EQ. 0.) GO TO 47
128 YSUM = YSUM + YTOT(M)
      IVAR = IVAR + 1
      IF (IVAR .EQ. 25 .OR. IVAR .EQ. 50) DMIN = 100.*DMIN
      IF (IVAR .EQ. 75) GO TO 59
      IF (IVARJ .LT. 0 .OR. L1 .EQ. 0 .OR. SLAM .LT. 1.) GO TO 16
      IVARJ = IVARJ + 1
      IF (IVARJ .EQ. 10) GO TO 88
      DO 3 N = 1, MPA
        M = IFAS(N)
        MA = MF(M)
        MB = ML(M)
        DO 3 I = MA, MB
          IF (Y(I) .GT. 0. .AND. DABS(YX(I))/Y(I) .GT. 1.E-6) GO TO 16
3  CONTINUE
88  DO 149 N = 1, MPA
      M = IFAS(N)
      CALL XBER
      IF (MA .NE. MB) GO TO 133
      DO 92 J = 1, L
        IF (A(MA,J) .NE. A0(MA,J)) Y(MA) = A(MA,J)/A0(MA,J)*Y(MA)
92  CONTINUE
133 DO 149 I = MA, MB
      IF (NO(I) .EQ. 0 .OR. Y(I) .GT. 0.) GO TO 149
      Y(I) = YTOI(M)*YF(I)
      IF (Y(I) .LT. 1.E-20 .OR. LX(I) .EQ. 1) GO TO 149
      LX(I) = 1
      GO TO 134
149 CONTINUE
      IF (IVARJ .EQ. 10) M = 0
      RETURN
      END

```

```

SUBROUTINE ABER
  IMPLICIT REAL*8 (A-H,O-Z)
  COMMON A(99,10), AO(99,10), AKT(99), AKTF(99), B(10,99), BO(10),
  $G(99), KH(20), L, N, M1, MA, MB, MF(20), ML(20), MP, MS, NO(99),
  $NP, PI(20), PTOT, T, TEXT(99), Y(99), YF(99), YTOT(20), V, NV, NVV
  YTOT(M) = 0.
  DO 2 I = MA, MB
2  YTOT(M) = YTCT(M) + Y(I)
  IF (YTOT(M) .GE. 1.E-8) GO TO 151
  YTOT(M) = 0.
  RETURN
151 CONTINUE
  IF (NV.EQ.0) GO TO 326
  YA=0.
  DO 325 I=1,ML(1)
325 YA=Y(I)+YA
  PTOT=YA*.0821*T/V
326 CONTINUE
  IF (M .EQ. 1) YTOT(1) = YTOT(1)/PTOT
  DO 127 I = MA, MB
127 YF(I) = Y(I)/YTOT(M)
  CALL FACTOR
  DO 141 I = MA, MB
141 AKT(I) = AKTF(I)*YF(I)
  RETURN
  END

```

```

SUBROUTINE XBER
  IMPLICIT REAL*8 (A-H,O-Z)
  COMMON A(99,10), AO(99,10), AKT(99), AKTF(99), B(10,99), BO(10),
  $G(99), KH(20), L, M, M1, MA, MB, MF(20), ML(20), MP, MS, NO(99),
  $NP, PI(20), PTOT, T, TEXT(99), Y(99), YF(99), YTOT(20), V, NV, NVV
  DIMENSION OYF(99)
  PLOG = DMAX1(DLOG(PTOT), 10.)
  MA = MF(M)
  MB = ML(M)
  DO 38 I = MA, MB
    IF (NO(I) .EQ. 0 .OR. Y(I) .GT. 0.) GO TO 38
    PIA = -G(I)
    DO 87 J = 1, L
      87 PIA = PIA + A(I,J)*PI(J)
    IF (PIA .GT. PLOG) PIA = PLOG
    AKT(I) =DEXP(PIA)
    YF(I) = AKT(I)
  38 CONTINUE
  IVAR = 0
  147 IVAR = IVAR + 1
  IF (IVAR .LT. 25) CALL FACTOR
  DO 139 I = MA, MB
    OYF(I) = YF(I)
  139 YF(I) = AKT(I)/AKTF(I)
  DO 137 I = MA, MB
    IF (YF(I) .GT. 0. .AND. DABS(OYF(I)/YF(I)-1.) .GT. 1.E-4) GO TO 147
  137 CONTINUE
  RETURN
END

```

```

SUBROUTINE FACTOR
IMPLICIT REAL*8 (A-H,O-Z)
COMMON A(99,10), AO(99,10), AKT(99), AKTF(99), B(10,99), BO(10),
$G(99), KH(20), L, M, M1, MA, MB, MP(20), ML(20), MP, MS, NO(99),
$NP, PI(20), PTOT, T, TEXT(99), Y(99), YF(99), YTOT(20), V, NV, NVV

```

```

C
C      THE ACTIVITY COEFFICIENT EXPRESSIONS FOR THE SPECIES IN THE NONIDEAL
C      MIXTURES ARE INSERTED AFTER THE STATEMENT NUMBER THAT CORRESPONDS TO
C      THE MIXTURE NUMBER. FOR A SOLID WITH VARIABLE STOICHIOMETRY WHICH IS
C      REGARDED AS A SEPARATE MIXTURE, THE COMPOSITION MUST ALSO BE SPECIFIED
C      (MAXIMUM ONE STOICHIOMETRIC COEFFICIENT IS ALLOWED TO DEVIATE).

```

```

C      NOTICE THAT AN AMOUNT OF A SPECIES WHICH IS LESS THAN 1.E-20 MOLES
C      IS SET EQUAL TO ZERO.

```

```

C      AO = A DEVIATING STOICHIOMETRIC COEFFICIENT
C      AKT = ACTIVITY
C      AKTF = ACTIVITY COEFFICIENT
C      Y = AMOUNT OF SUBSTANCE
C      YF = MOLE FRACTION OR PARTIAL PRESSURE
C

```

```

      GO TO (1,2,3,4,5,6,7,8,9,10), M
1 CONTINUE
  RETURN
2 CONTINUE
  RETURN
3 CONTINUE
  RETURN
4 CONTINUE
  RETURN
5 CONTINUE
  RETURN
6 CONTINUE
  RETURN
7 CONTINUE
  RETURN
8 CONTINUE
  RETURN
9 CONTINUE
  RETURN
10 CONTINUE
  RETURN
  END

```

```

SUBROUTINE SPEQUA
  IMPLICIT REAL*8 (A-H,O-Z)
  COMMON A(99,10), AO(99,10), AKT(99), AKTF(99), B(10,99), BO(10),
  $G(99), KH(20), L, M, M1, MA, MB, MF(20), ML(20), MP, MS, NO(99),
  $NP, PI(20), PTOT, T, TEXT(99), Y(99), YF(99), YTOT(20), V, NV, NVV

```

```

C
C      SPEQUA IS A SUBROUTINE FOR CALCULATION OF QUANTITIES WHICH ARE
C      DERIVABLE FROM THE EQUILIBRIUM COMPOSITION.
C

```

```

  RETURN
  END

```


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