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IS-1693

Chemistry (UC-4)
TID-4500, March 1, 1967

UNITED STATES ATOMIC ENERGY COMMISSION

Research and Development Report

COMPUTER PROGRAM FOR INTER-
PRETATION OF SPARK SOURCE
MASS SPECTROGRAPH PHOTOPLATES

by

R. J. Conzemius, D. H. Erbeck and
S. T. Elbert

October 1967

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Printed in the United States of America

Available from

Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U. S. Department of Commerce
Springfield, Virginia 22151

Price: Printed Copy \$3.00; Microfiche \$0.65

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IS-1693

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COMPUTER PROGRAM FOR INTERPRETATION OF SPARK
SOURCE MASS SPECTROGRAPH PHOTOPLATES

R. J. Conzemius, D. H. Erbeck* and S. T. Elbert

ABSTRACT

A method is described which takes raw data from a spark source mass spectrograph photoplate and utilizes computer techniques for both interpretation and computation of elemental impurity levels. A general description of the program is provided as well as a block diagram and complete listing. An example shows the type of input and output data. Limitations of the method are discussed briefly.

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INTRODUCTION

The mass spectrum of a sample ionized in the high frequency spark is generally displayed as a series of lines on a photoplate. However, since the ion optic systems of real mass spectrographs do not permit infinite resolution of all ions of all possible masses, each line may include contributions from a number of sources. These may include singly charged nuclides of different elements whose exact masses differ slightly because of their packing fractions, multiply charged nuclides and multi-atom ions of various charges. The problem of manually handling such diverse data is a formidable one in many cases.

The utilization of computer techniques to interpret mass spectra is finding wide acceptance. For example, they have become especially popular in interpreting high resolution organic mass spectra.^{1, 2} Computers have been used in conjunction with data obtained from the spark source mass spectrograph.³⁻⁵ However, their usage with these data has been restricted mainly to data reading, mass calculations, photoplate emulsion calibrations, and arithmetic computations. A computer program which is used to interpret the spectra as well as perform these other functions is described here.

Methods of interpreting spark source spectra can generally be described mathematically because the nature of the data (isotope abundances, probability of multiple charging, atom clustering, line intensities, exposure levels, etc.) permits establishment of sufficient equations to allow for determining abundances for each species. In some cases the

spectrum can be so simple that visual interpretation is adequate for almost complete interpretation. In other cases the spectrum is complicated (e. g., inorganic salts) and interpretation becomes considerably more difficult and time consuming. This computer program was written to interpret completely data obtained directly from a photographic plate. However, provisions were made to allow the densitometer operator to insert as much information as his experience allows. The program performs only computational tasks if all features of the spectrum have been completely identified. It will also perform interpretation tasks if features in the spectrum have been only partially identified.

The program has been tested for approximately one year. It has worked well and because of its "modular" format, has been readily updated to accommodate changes in hardware and data handling. The applicability of this program to computers other than the IBM-360-50 may be limited due to core size.

No attempt will be made here to describe the program completely, due to lack of space. Instead, the general method will be described first, followed by a block diagram, complete listing, and a definition of variables (arranged alphabetically by subroutine). An actual example will be given and this will be followed by a summary which describes present limitations and further planned development.

GENERAL EXPLANATION

The objective of the program is to process raw spark source mass spectrographic data which is normally recorded on a photographic plate and consists of optical transmissions, relative line widths, exposure values, and an indication of mass either in the form of a rough approximation or a relative position measurement.

CALCULATIONS

Calibration curve. Correlation of transmission to relative line intensity is obtained with a photoemulsion calibration curve. This program currently uses a modified Churchill 2-line method for the calibration. Data from various sets of isotopes are plotted manually to obtain a best fit for the calibration curve. The isotopic ratios are corrected for line width and mass effect. A set of transmission values is read from the calibration curve for a particular isotopic ratio and this information is inserted into the input data. The computer first forms a preliminary curve and from it forms the calibration curve by using a four point Lagrangian interpolation. This interpolation scheme is also used to read relative intensity values from the calibration curve for the transmission values of the spectral lines.

Reference intensity. The relative concentration of the internal standard is inserted by the densitometer operator. He also identifies and reads raw data for the lines of the internal standard. An average value of intensity-to-exposure ratio is computed for the internal standard

lines. This average is used along with the relative concentration of the internal standard to calculate the remaining spectral line intensities.

Mass - position scale. If the mass is not recorded for a particular line, then the position of the line is used to obtain the mass. A mass versus position scale is established at this point by reading in known masses along with their respective positions. From this scale any position data will be changed to mass by utilizing a two point Lagrangian interpolation.

Spectral line intensities. Relative intensities for each spectral line are calculated in the manner described by Owens and Giardino⁶ (MASP Statement No. 466). After being tested by a rejection criterion, an average value, average deviation, and percent average deviation are calculated for each mass. A standard upper limit value is also calculated in the same manner for clear regions of the plate.

INTERPRETATION

The computer is confronted with the problem of determining what caused the lines and making corrections for interferences. The process is divided into three major steps. Step one is labeled Gross Equations and consists of a listing of equations representing each line on the photoplate. The left hand side of each equation gives the intensity of a given line. The right hand side lists the ions (in order of increasing mass) whose mass-to-charge ratio is within the uncertainty of a given mass represented by a line. Multiply charged ions are not listed unless pertinent lesser charged masses are observed with a particular

relative intensity. Step two is labeled Net Equations and consists of a relisting of the Gross Equations with an important exception. Prior to this listing all the possible ions shown in the Gross Equations are subjected to a series of tests which determine if the ion can contribute more than 10%* to the intensity of the line. If an ion fails this test, it does not appear in the second listing and is replaced by a coded explanation indicating which test proved that the ion contributed less than 10% to the intensity. The third step is labeled Solved Equations and is a listing of the solution of the Net Equations in terms of concentration per unit abundance of each ion.

Gross Equations. In generating the gross equations matrix, the computer has available in its memory the precise mass and abundance of 291 naturally occurring nuclides. Each nuclide whose mass falls within the uncertainty range associated with each line (either calculated from mass-position data or given directly) is considered a possible ion for that mass. Careful use of the mass uncertainty factor is mandatory to allow for specific and yet complete assignment of ions to lines.

The presence of multiply charged ions for each nuclide is determined by dividing the mass of each nuclide by the possible number of charges and determining whether or not any of these values fit the mass range of the spectral line in question. The listing of ions with multiple charges includes only those ions whose intensities decrease by at least a factor of two when compared with that of an ion of lesser charge. This criterion can be made regardless of the composition of the ion due to the

*This "10%" figure represents the uncertainty level generally associated with the line intensities.

expected decrease in intensity with increased charge. Thus, the computer searches the spectrum and investigates which multiply charged lines show sufficient intensity at a lesser charge. The search for multiply charged ions is investigated up to any charge indicated in the input, LC for elemental ions, 3 for molecular ions, and LCS for the main constituent.

Molecular ions (sometimes called clusters) whose presence is suspected may be included in the computer's memory along with the nuclides by writing each ion's symbol into the input data. The masses and abundances of every combination of the constituent isotopes are found automatically and these data are incorporated into the computer's memory along with the simple nuclides. This provision is particularly useful when hydrocarbon lines are present and when the spectrum has many clusters from the major components of the sample.

In order to avoid overlooking a possible cluster, the program also generates "unnamed clusters". Such clusters are found by searching lines representing lesser masses for a sum which falls within the uncertainty of a given line. These clusters will appear in the Gross Equations if the product of the intensities of their constituent masses is 10^7 times the concentration of the given line. This occurs only when there are no clusters with constituent masses equal to the two masses forming the required sum. The "unnamed cluster" is assigned an arbitrary abundance of unity and a symbol containing the two constituent masses.

The Gross Equations are written in order of increasing mass, except when the densitometer operator is certain a line is due to a specific ion. In this case the operator "names" the mass of that line with the ion's symbol and the computer will not consider other possible ions. These masses along with the named ions will appear at the beginning of the Gross Equations (before the unnamed masses).

Net Equations. At this point the computer is told in which of two forms the data have been inserted. In the first form, the computer assumes that all observable lines were recorded and will make decisions on the basis that all information is available. The second form represents a partial recording of the data and the computer makes no assumptions regarding data not recorded.

Each ion listed in the Gross Equations is subjected to a series of "tests" to determine if it contributes to the spectrum. The initial test is to compare isotopes of the same element. All isotopes whose abundances are within a factor of ten of each other are compared and any one can cause an elimination on the basis of the above test. A check is also made for all isotopes with a lesser charge if necessary. In this case a decrease in intensity by a factor of two is assumed for each additional charge.

Any cluster that contains hydrogen is subjected to a test which is based upon the high fragmentation observed in the spark spectra. This test consists of comparing the concentration at the mass of the cluster in question with concentration at that mass minus a hydrogen mass.

If the concentration at one less hydrogen mass unit is less than 10% of the concentration at the mass of the hydride, the cluster is rejected.

Multiplets (spectra lines with the same nominal mass) may be given the same mass in the input data. In the Gross Equation listing, all the ions will appear with the lowest mass of the multiplet. In this case the testing procedure is arranged to make maximum use of the relative position of the ion in order of mass with respect to the intensity data. If after completing the test section there remain exactly as many possible ions as lines in the multiplet, the ions are assigned to the masses in order of their weight. If there are fewer possible ions than lines in the multiplet, the ions are assigned to the lower masses and the remaining line or lines in the multiplet are ignored but a statement is printed out concerning this fact. If there are more ions than lines, the ions closest in mass are combined until the number of ion groups is the same as the number of lines in the multiplet and the groups are then assigned to their respective masses.

After completing these tests for each ion, the results are printed under the heading Net Equations in the same format as the Gross Equations with the exception that the eliminated ions are simply replaced by numbers indicating why they were eliminated. This matrix now contains all the information on line intensity and positive ions contributing to the intensity.

Matrix Solution. The program has been written to allow for up to 300 equations. If as many unknowns as equations exist, this would

require a huge storage if a square matrix was used. However, since most of the square matrix is empty (i. e. a banded matrix), a technique was devised to handle this problem. The technique will be described in more detail in the section "Definition of Variables" since it also has some general applicability to other problems in the solution of large matrices.

FINAL COMPUTATIONS

The final portion of the program consists of computations which list the symbol and charge state for each element along with its concentration in ppm atomic and ppm by weight. This is done in two general forms. The first assumes unit sensitivities for all the elements. The second form makes use of relative sensitivities which places the data on a quantitative basis for cases where the sensitivities have been established. Relative sensitivities can be changed if desired by inserting the elemental symbol and its changed sensitivity into the input data.

TECHNICAL DESCRIPTION OF PROGRAM

Block Diagram of Main Program.

Listing

```

COMMON/TABLE/SENS(88),ATWT(88),ISYM(88),TAIN(700),TMC(700),MS(700) MASP 10
COMMON UM(300),CIN(300),CL1(400),CL2(400),CLM(400),CLA(400), MASP 20
C    UN(500),UMN(500),UCI(500),LGO,BLANK,UL1,NMC,AIN(300,15) MASP 30
DIMENSION TL(25),TD(25),TDN(25),R(25),TP(25),TB(25),W(25),E(25), MASP 40
D    ANC(25),AIP(25),AIR(25),EDVN(25),SQRTMS(25),POS(25),C(25), MASP 50
D    IUN(25),NN(25),TM(100),TA(100),LCL1(60),LCL2(60),IIE(25), MASP 60
D    XLAB(5),YLAB(5),GLAB(5),DLAB(5),PLTDN(25),RLOG(25), MASP 70
D    REMKS(5),UN1(101),NT1(101),NT2(101),IC(101),COMNT(7) MASP 80
DIMENSION WIN(2000) MASP 90
DIMENSION IAN(300,15) MASP 100
EQUIVALENCE (AIN(1,1),IAN(1,1)) MASP 110
INTEGER*2 IN(300,15),LIN(2000) MASP 120
INTEGER BLANK,CL1,CL2 MASP 130
MAXMS=700 MASP 140
MAXCL=400 MASP 150
BLANK=1077952576 MASP 160
NC=15 MASP 170
DO 16 I=1,291 MASP 180
16  TAIN(I)=TAIN(I)/100. MASP 190
C          CALCULATE CURVES MASP 200
C MASP 210
READ(1,1)NTE,N,RO,TD1,PLT MASP 220
FORMAT(2I10,3F10.0) MASP 230
1  READ(1,2)(TL(NE),TD(NE),NE=1,NTE) MASP 240
2  FORMAT(8E10.0) MASP 250
NP1=N+1 MASP 260
TDN(NP1)=TD1 MASP 270
R(NP1)=1. MASP 280
DO 20 II=2,NP1 MASP 290
I=N+2-II MASP 300
CALL INTERP(TL,TD,NTE,4,TD1,TD2) MASP 310
IF(TD2-TD1)18,17,17 MASP 320
17  KK=17 MASP 330
GO TO 89 MASP 340
18  TDN(I)=TD2 MASP 350
TD1=TD2 MASP 360
20  R(I)=RO**((II-1)) MASP 370
C          PLOT CALIBRATION CURVE MASP 380
IF(PLT)22,274,22 MASP 390
22  READ(1,24)XLAB,YLAB,GLAB,DLAB MASP 400
24  FORMAT(20A4) MASP 410
CALL LABEL('A0163MASP') MASP 420
PAUSE ' USE LOG-X LINEAR-Y PLOT PAPER 00' MASP 440
DO 26 I=1,NP1 MASP 450
J=NP1-I+1 MASP 460
RLOG(J)=ALOG10(R(I))*7.5+7.5 MASP 470
26  PLTDN(J)=TDN(I)/10. MASP 480
X1=ALOG10(.5)*7.5+7.5 MASP 490
X2=ALOG10(50000.)*7.5+7.5 MASP 500
CALL AXIS(X1,0,YLAB,20,10.,90.,0,10.,10.) MASP 510
CALL SYMBOL(11.5,-.4,.2,XLAB,C,20) MASP 520
IZ=3 MASP 530
X3=(X2-X1)/100 MASP 540
X4=X1-X3 MASP 550
DO 27 I=1,101 MASP 560
X4=X4+X3 MASP 570
CALL INTERP(RLOG,PLTDN,NP1,4,X4,Y4) MASP 580
CALL PLOT(X4,Y4,IZ) MASP 590
27  IZ=2 MASP 600
PLTDN(NP1+2)=1. MASP 610

```

	RLOG(NP1+2)=1.	MASP 620
	CALL LINE(RLOG,PLTDN,NP1,1,- 1,3)	MASP 630
	XX=11.	MASP 640
	YY=9.	MASP 650
	CALL SYMBOL(XX,YY,,2,GLAB,0,4C)	MASP 660
	CALL ENDPLT	MASP 670
C		MASP 680
	CALCULATE STANDARD	MASP 690
C		MASP 700
274	DO 275 I=1,NP1	MASP 710
275	R(I)=ALOG10(R(I))	MASP 720
	IUP=NP1	MASP 730
28	READ(1,3)NE ,SMASS,AIS,SS,NAME,LCS,STMAS,REMK	MASP 740
3	FORMAT(110,3F10.0,A4,12,4X,F10.0,5A4)	MASP 750
	IF(NC)1000,1000,285	MASP 760
285	CALL ZERO(IN,150*NC)	MASP 770
	CALL ZERO(AIN,300*NC)	MASP 780
	CALL ZERO(LIN,1000)	MASP 790
	CALL ZERO(WIN,2000)	MASP 800
	READ(1,2)(E(I),I=1,NE)	MASP 810
	I=0	MASP 820
295	I=I+1	MASP 830
	READ(1,6)TP(I),TB(I),W(I),IE, LAST	MASP 840
	CALL INTERP(TDN,R,IUP,4,TP(I),AIP(I))	MASP 850
	CALL INTERP(TCN,R,IUP,4,TB(I),AIB(I))	MASP 860
	ANC(I)=(10.**AIP(I)-10.**AIB(I))*W(I)	MASP 870
30	EOVN(I)=E(IE)/ANC(I)	MASP 880
	IF(LAST)31,295,31	MASP 890
31	NEXP=I	MASP 900
	SUM =0.	MASP 910
	DO 35 I=1,NEXP	MASP 920
35	SUM=SUM+ EOVN(I)	MASP 930
	FI=NEXP	MASP 940
	EOVNS=SUM/FI	MASP 950
	SUM=0.	MASP 960
	DO 37 I=1,NEXP	MASP 970
37	SUM =SUM+ABS(ECVN(I)-EOVNS)	MASP 980
	AVDEV=SUM/FI	MASP 990
	PCDEV=100.*AVDEV/EOVNS	MASP1000
	WRITE(3,101)NTP,N,RO,TD1	MASP1010
101	FORMAT(11H1.19X20HCAI TTRATION CURVE -5X15,5X15,5XF10.5,5XF10.5)	MASP1020
	WRITE(3,8)NEXP,SMASS,AIS,SS,NAME,LCS,STMAS,REMK	MASP1030
8	FORMAT(//13X11HSTANDARD -5X,15,5XF10.5,5XF10.5,5XF10.5,5X	MASP1040
	A4,'+'12,2X,F10.5,5X,5A4)	MASP1050
	WRITE(3,4)EOVNS,AVDEV,PCDEV	MASP1060
4	FORMAT(//20X16HAVERAGE ES/NSC =E15.8,5X19HAVERAGE DEVIATION = ,	MASP1070
	4 E15.8,5X9HPCT DEV =F7.2)	MASP1080
	WRITE(3,10)(EOVN(I),I=1,NEXP)	MASP1090
10	FORMAT(/21X6E15.8)	MASP1100
C		MASP1110
	CALCULATE DEFAULT ATTRIBUTE3	MASP1120
C		MASP1130
	NEQ=0	MASP1140
	NIN=0	MASP1150
40	READ(1,102)LGC,NM,SUNC,SUNC1,SPUNC,SPUNC1,LC,TP(1),TR(1),W(1),IE	MASP1160
102	FORMAT(11,14,5X,2(F10.0,1XF8.4),15,5X,3E10.7,12)	MASP1170
	TBS=TB(1)	MASP1180
	IES=IE	MASP1190
	SUNC=SUNC/SUNC1	MASP1200
	SPUNC=SPUNC/SPUNC1	MASP1210
41	IF(SPUNC)415,41,415	MASP1220
415	SPUNC=SPUNC1	
	CALL INTERP(TCN,R,IUP,4,TP,AIP)	

```

CALL INTERP(TCN,R,IUP,4,TB,AIB)
ANC(1)=(10.**AIP(1)-10.**AIB(1))*W(1)
UL1=EQVNS *AIS *ANC(1)*1.E+6/(E(IE)*SQRT(SMASS)**3)
WRITE(3,42)UL1
42  FORMAT('0'10X'DEFAULT UPPER LIMIT IS'F10.6/)
    IF(NM)43,44,43
43  READ(1,2)(SQRTMS(I),POS(I),I=1,NM)
    DO 435 I=1,NM
435  SQRTMS(I)=SQRT(SQRTMS(I))
C                                     CALCULATE IMPURITIES
44  J=0
    NTEQ=0
    WRITE(3,445)
445  FORMAT('0 MASS COMNT'7X'FCT DEV AVG C(I)'9X'C(I)S VS EXP')
45  J=J+1
    READ(1,5)UMASS,UNC1,UNC,PSN,NAM1,NAM2,ICG,TP(1),TB(1),W(1),IE,
5    COMNT, LAST
5  FORMAT(F10.7,F1.0,1XF8.4,F10.7,2A4,I2, 3F10.7,I2,7A1,I1)
    IF(TB(1))453,452,453
452  TB(1)=TBS
453  IF(IE)455,454,455
454  IE=IES
    LAST=1
455  IF(UMASS)456,49,4917
C                                     FROM MASS, TO MASS, UP.LIM. IF NOT STANDARD UP.LIM.
456  UMN(J)=UMASS
    UMN(J+1)=-UNC
    UN(J)=-SUNC*UMASS
    UN(J+1)=UN(J)
    IF(TP(1))46,47,46
46  CALL INTERP(TCN,R,IUP,4,TP,AIP)
    CALL INTERP(TCN,R,IUP,4,TB,AIB)
    IF(W(1))466,464,466
464  W(1)=UNC
466  ANC(1)=(10.**AIP(1)-10.**AIB(1))*W(1)
    UCI(J)=EQVNS *SQRT(-UMASS/SMASS)*AIS *(ANC(1)/E(IE))*1.E+6
    UCI(J+1)=0.
    GO TO 48
47  UCI(J)=UL1*SQRT(-UMASS)**3
    UCI(J+1)=0.
    J=J+1
    WRITE(3,482)UMN(J-1),UMN(J),UCI(J-1),COMNT
482  FORMAT(10X'NEGATIVE FROM MASS'F7.2,' TO MASS'F7.2,' UP.LIM.'F9.2,
F 5X7A1)
    GO TO 45
C                                     NOM MASS, UNCERTAINTY, OPT PSN, OPT NAME
49  IF(PSN)52,52,491
491  CALL INTERP(POS,SQRTMS,NM, 2,PSN,UMASS)
    UMASS=UMASS*UMASS
    IF(UNC)4913,4916,4913
4913  IF(UNC1)4914,4915,4914
4914  UN(J)=(UNC1/UNC)*UMASS/PSN
    GO TO 492
4915  UN(J)=UNC*UMASS/PSN
    GO TO 492
4916  UN(J)=SPUNC*UMASS/PSN
    GO TO 492
4917  IF(UNC)4918,4919,4918
4918  IF(UNC1)49185,49183,49185
49183  UN(J)=UNC*UMASS
    GO TO 492

```

```

MASP1230
MASP1240
MASP1250
MASP1260
MASP1270
MASP1280
MASP1290
MASP1300
MASP1310
MASP1320
MASP1330
MASP1340
MASP1350
MASP1360
MASP1370
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MASP1640
MASP1650
MASP1660
MASP1670
MASP1680
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MASP1770
MASP1780
MASP1790
MASP1800
MASP1810
MASP1820
MASP1830

```

49185	UN(J)=UNC1/UNC*UMASS	MASP1840
	GO TO 492	MASP1850
4919	UN(J)=SUNC*UMASS	MASP1860
492	SUM=0.	MASP1870
	NTEQ=NTEQ+1	MASP1880
	I=1	MASP1890
	GO TO 4968	MASP1900
496	I=I+1	MASP1910
	READ(1,6) TP(1),TB(1),W(1),IE,LAST	MASP1920
6	FORMAT(40X2F10.7,F10.7,I2,7X11)	MASP1930
	IF(TB(1))4962,4962,4963	MASP1940
4962	TB(1)=TBS	MASP1950
4963	IF(IE)4968,4964,4968	MASP1960
4964	IE=IES	MASP1970
	LAST=1	MASP1980
4968	IF(W(1))498,497,498	MASP1990
497	W(1)=UMASS	MASP2000
498	CALL INTERP(TCN,R,IUP,4,TP,AIP)	MASP2010
	CALL INTERP(TCN,R,IUP,4,TB,AIB)	MASP2020
	ANC(I)=(I11.**AIP(1)-10.**AIB(1))+W(1)	MASP2030
	C(I)=ECVNS *SORT(UMASS/SMASS)*AIS *ANC(1)*1.E+6/E(IE)	MASP2040
	IIE(I)=IE	MASP2050
	SUM=SUM+C(I)	MASP2060
	IF(LAST)50,496,50	MASP2070
50	F=1	MASP2080
	AVG=SUM/FI	MASP2090
	NEXP=I	MASP2100
	DO 504 I=1,NEXP	MASP2110
	IF(ABS((C(I)-AVG)/AVG)-.5)504,504,502	MASP2120
502	AVG=(AVG*FI-C(I))/(FI-1.)	MASP2130
	C(I)=-C(I)	MASP2140
	FI=FI-1.	MASP2150
504	CONTINUE	MASP2160
	SUM=0.	MASP2170
	DO 5046 I=1,NEXP	MASP2180
	IF(C(I))5046,5046,5045	MASP2190
5045	SUM=SUM+ABS(C(I)-AVG)	MASP2200
5046	CONTINUE	MASP2210
	PCTDV=100.*SUM/FI /AVG	MASP2220
	WRITE(3,505)UMASS,COMNT,PCTDV,AVG,(C(I),IIE(I),I=1,NEXP)	MASP2230
505	FORMAT(F10.3,1X7A1,1X2F12.3,5X,5(F12.3,I3)/25X7(F12.3,I3)/	MASP2240
	F 25X7(F12.3,I3))	MASP2250
	IF(NAM1-BLANK)508,506,508	MASP2260
506	UMN(J)=UMASS	MASP2270
	UCI(J)=AVG	MASP2280
	GO TO 45	MASP2290
508	NIN=NIN+1	MASP2300
	NEQ=NEQ+1	MASP2310
	CIN(NEQ)=AVG	MASP2320
	AIN(NEQ,1)=1.	MASP2330
	IN(NEQ,1)=NIN	MASP2340
	NT1(NEQ)=NAM1	MASP2350
	NT2(NEQ)=NAM2	MASP2360
	IC(NEQ)=ICG	MASP2370
	UM(NEQ)=UMASS	MASP2380
	UN1(NEQ)=UN(J)	MASP2390
	UCI(J)=AVG	MASP2400
	UMN(J)=-UMASS	MASP2410
	UMN(J+1)=-UMASS	MASP2420
	J=J+1	MASP2430
	GO TO 45	MASP2440

C	SET UP ION TABLES ADDITIONS	MASP2450
52	IGC=1	MASP2460
	IF(NTEQ-300)524,524,522	MASP2470
522	WRITE(3,523)NTEQ	MASP2480
523	FORMAT(110,' LINES EXCEEDS MAXIMUM OF 300')	MASP2490
	KK=522	MASP2500
	GO TO 89	MASP2510
524	NNAM=NEQ	MASP2520
	NMC=J-1	MASP2530
	NIT=291	MASP2540
	READ(1,525)NCLC,NCL,NSENS	MASP2550
525	FORMAT(8110)	MASP2560
	K=0	MASP2570
	IF(NCLC)575,575,53	MASP2580
53	DO 57 I=1,NCLC	MASP2590
	READ(1,7)NCL1,N1,NCL2,N2,(ION(J),J=1,14)	MASP2600
7	FORMAT(A3,I2 ,A3,I2 ,14(A4,1X))	MASP2610
54	DO 55 J=1,NIT	MASP2620
	IF(MS(J)-NCL1)55,551,55	MASP2630
55	CONTINUE	MASP2640
5505	KK=55	MASP2650
	WRITE(3,5506)NCL1,NCL2	MASP2660
5506	FORMAT(' CLUSTER COMPONENT 'A4,' OR 'A4,' HAS NOT BEEN COMPUTED')	MASP2670
	GO TO 89	MASP2680
551	J1=J	MASP2690
	IF(N2)5562,5562,552	MASP2700
552	DO 555 J=1,NIT	MASP2710
	IF(MS(J)-NCL2)555,556,555	MASP2720
555	CONTINUE	MASP2730
	GO TO 5505	MASP2740
556	J2=J	MASP2750
5562	N3=N1+N2	MASP2760
	DO 5564 J=1,N1	MASP2770
5564	NN(J)=J1	MASP2780
	N2=N1+1	MASP2790
	DO 5566 J=N2,N3	MASP2800
5566	NN(J)=J2	MASP2810
557	K1=NN(1)-1	MASP2820
5571	K1=K1+1	MASP2830
	IF(MS(K1+1)-MS(K1))5572,5571,5572	MASP2840
5572	DO 57 N=2,N3	MASP2850
	K2=NN(N)-1	MASP2860
5573	K2=K2+1	MASP2870
	IF(MS(K2+1)-MS(K2))5574,5573,5574	MASP2880
5574	L=0	MASP2890
	NNM1=NN(N-1)	MASP2900
	NNN=NN(N)	MASP2910
	DO 558 L1=NNM1,K1	MASP2920
	DO 558 L2=NNN,K2	MASP2930
	L=L+1	MASP2940
	TM(L)=TMC(L1)+TMC(L2)	MASP2950
558	TA(L)=ABS(TAIN(L1)*TAIN(L2))	MASP2960
	A=TAIN(K1)	MASP2970
	B=TAIN(K2)	MASP2980
	SGN=SIGN(1.,SIGN(1.,A*B)+SIGN(1.,A)+SIGN(1.,B))	MASP2990
	IF(L-100)5583,5583,5582	MASP3000
5582	KK=5582	MASP3010
	WRITE(3,55825)NCL1,NCL2	MASP3020
55825	FORMAT(' CLUSTER COMPONENTS 'A4,' AND 'A4,' HAVE A PRODUCT OF MORE THAN 100 ISOTOPES')	MASP3030
	GO TO 89	MASP3040
		MASP3050

5583	LM1=L-1	MASP3060
	DO 5602 L1=1,LM1	MASP3070
	IF(TA(L1))5585,5602,5585	MASP3080
5585	L1P1=L1+1	MASP3090
	DO 560 L2=L1P1,L	MASP3100
	IF(ABS(TM(L1)-TM(L2))-1)559,560,560	MASP3110
559	TM(L1)=(TA(L1)*TM(L1)+TA(L2)*TM(L2))/(TA(L1)+TA(L2))	MASP3120
	TA(L1)=TA(L1)+TA(L2)	MASP3130
	TM(L2)=0.	MASP3140
	TA(L2)=0.	MASP3150
560	CONTINUE	MASP3160
5602	CONTINUE	MASP3170
	GO TO(5605,582),IGG	MASP3180
5605	NN(N)=NIT+1	MASP3190
	DO 566 L1=1,L	MASP3200
	AMAX=0.	MASP3210
	IT=0	MASP3220
	DO 563 L2=1,L	MASP3230
	IF(TA(L2)-AMAX)563,563,561	MASP3240
561	AMAX=TA(L2)	MASP3250
	IT=L2	MASP3260
563	CONTINUE	MASP3270
	IF(AMAX-1.E-5)568,568,565	MASP3280
565	NIT=NIT+1	MASP3290
	MS(NIT)=ION(N-1)	MASP3300
	TAIN(NIT)=TA(IT)*SGN	MASP3310
	TMC(NIT)=TM(IT)	MASP3320
	TA(IT)=0.	MASP3330
566	CONTINUE	MASP3340
568	K1=NIT	MASP3350
57	CONTINUE	MASP3360
	IF(NIT-MAXMS)575,575,572	MASP3370
572	WRITE(3,573)NIT,MAXMS	MASP3380
573	FORMAT(I10,' CLUSTER COMPONENTS EXCEEDS MAX CF 'I5)	MASP3390
	KK=572	MASP3400
	GO TO 89	MASP3410
C	FORMATION OF NAMED CLUSTERS	MASP3420
575	IF(NCL)5925,5925,576	MASP3430
576	IGO=2	MASP3440
	I=0	MASP3450
	K=0	MASP3460
	READ(1,9)(LCL1(J),LCL2(J),J=1,NCL)	MASP3470
9	FORMAT(8(2A4,2X))	MASP3480
	GO TO 592	MASP3490
58	I=I+1	MASP3500
	IF(LCL2(I)-BLANK)581,5801,581	MASP3510
5801	DO 5802 J=1,NIT	MASP3520
	IF(MS(J)-LCL1(I))5802,5803,5802	MASP3530
5802	CONTINUE	MASP3540
	KK=58	MASP3550
	GO TO 89	MASP3560
5803	K=K+1	MASP3570
	CL1(K)=LCL1(I)	MASP3580
	CL2(K)=BLANK	MASP3590
	CLM(K)=TMC(J)	MASP3600
	CLA(K)=TAIN(J)	MASP3610
	J=J+1	MASP3620
	IF(MS(J)-MS(J-1))592,5803,592	MASP3630
581	N2=1	MASP3640
	NCL1=LCL1(I)	MASP3650
	N1=1	MASP3660

	NCL2=LCL2(I)	MASP3670
	GO TO 54	MASP3680
582	DO 59 L1=1,L	MASP3690
	AMAX=0.	MASP3700
	IT=0	MASP3710
	DO 586 L2=1,L	MASP3720
	IF(TA(L2)-AMAX)586,586,584	MASP3730
584	AMAX=TA(L2)	MASP3740
	IT=L2	MASP3750
586	CONTINUE	MASP3760
	IF(AMAX)588,592,588	MASP3770
588	K=K+1	MASP3780
	CL1(K)=NCL1	MASP3790
	CL2(K)=NCL2	MASP3800
	CLM(K)=TM(IT)	MASP3810
	CLA(K)=TA(IT)*SGN	MASP3820
	TA(IT)=0.	MASP3830
59	CONTINUE	MASP3840
592	IF(I-NCL)58,5925,5925	MASP3850
C	FORMATION OF UNNAMED CLUSTERS	MASP3860
5925	NUN=K	MASP3870
	DO 598 I=2,NMC	MASP3880
	IM1=I-1	MASP3890
	IF(UMN(I)-UMN(I-1))59254,598,59254	MASP3900
59254	CON=UCI(I)	MASP3910
	J=I	MASP3920
59255	J=J+1	MASP3930
5926	IF(UMN(I)-UMN(J))5929,5927,5929	MASP3940
5927	IF(UCI(J)-CON)5928,59255,59255	MASP3950
5928	CON=UCI(J)	MASP3960
	GO TO 59255	MASP3970
5929	DO 597 J=1,IM1	MASP3980
	J1=I	MASP3990
593	J1=J1-1	MASP4000
	IF(J1-J)597,5935,5935	MASP4010
5935	CONTINUE	MASP4020
5936	SUM=UMN(J)+UMN(J1)	MASP4030
	IF(SUM-UMN(I)-UMN(I))594,594,593	MASP4040
594	IF(ABS(SUM-UMN(I))-UN(I))5945,5945,597	MASP4050
5945	IF(UCI(J)*UCI(J1)-1.E+7*CON)593,595,595	MASP4060
C	IS POSSIBLE UNNAMED CLUSTER ACTUALLY A NAMED CLUSTER?	MASP4070
595	DO 5963 I1=1,NUN	MASP4080
	IF(ABS(SUM-CLM(I1))-UN(I))5951,5951,5963	MASP4090
5951	T1=UMN(J)	MASP4100
	UNJ=UN(J)	MASP4110
	SW1=0.	MASP4120
	DO 5952 I2=1,NIT	MASP4130
	IF(MS(I2)-CL1(I1))5952,5953,5952	MASP4140
5952	CONTINUE	MASP4150
5953	DO 5954 I3=1,NIT	MASP4160
	IF(MS(I3)-CL2(I1))5954,5955,5954	MASP4170
5954	CONTINUE	MASP4180
5955	I4=I2-1	MASP4190
5956	I4=I4+1	MASP4200
	IF(MS(I4)-MS(I2))5961,5957,5961	MASP4210
5957	IF(ABS(T1-TMC(I4))+TMC(I5)-UMN(I))5958,5958,5956	MASP4220
5958	I5=I3-1	MASP4230
5959	I5=I5+1	MASP4240
	IF(MS(I5)-MS(I3))5956,5960,5956	MASP4250
5960	IF(ABS(TMC(I4)+TMC(I5)-UMN(I))593,593,5959	MASP4260
5961	IF(SW1)59625,5962,59625	MASP4270

5962	T1=UMN(J1)	MASP4280
	UNJ=UN(J1)	MASP4290
	SW1=1.	MASP4300
	GO TO 5955	MASP4310
59625	CONTINUE	MASP4320
5963	CONTINUE	MASP4330
	K=K+1	MASP4340
	NOM=10.*UMN(J)	MASP4350
	CL1(K)=ILF(NOM)	MASP4360
	NGM=10.*UMN(J1)	MASP4370
	CL2(K)=ILF(NGM)	MASP4380
	CLM(K)=SUM	MASP4390
	CLA(K)=1.	MASP4400
	GO TO 593	MASP4410
597	CONTINUE	MASP4420
598	CONTINUE	MASP4430
C	SET NAMED MASSES	MASP4440
599	IF(NEQ)612,612,5995	MASP4450
5995	DO 61 I=1,NEQ	MASP4460
	IF(IC(I))5997,5997,5999	MASP4470
5997	IC(I)=1	MASP4480
5999	IF(NT2(I)-BLANK)604,600,604	MASP4490
600	DO 601 J=1,NIT	MASP4500
	IF(NT1(I)-MS(J))601,6002,601	MASP4510
6002	IF(ABS(UM(I)-TMC(J)/IC(I))-UN1(I))602,602,601	MASP4520
601	CONTINUE	MASP4530
	GO TO 604	MASP4540
602	LIN(I)=1000*IC(I)+J	MASP4550
	WIN(I)=0.	MASP4560
	AIN(I,1)=TAIN(J)	MASP4570
	GO TO 61	MASP4580
604	DO 606 J=1,K	MASP4590
	IF(NT1(I)-CL1(J))606,605,606	MASP4600
605	IF(NT2(I)-CL2(J))606,6052,606	MASP4610
6052	IF(ABS(UM(I)-CLM(J)/IC(I))-UN1(I))607,607,606	MASP4620
606	CONTINUE	MASP4630
	KK=606	MASP4640
	WRITE(3,6064)NT1(I),NT2(I),IC(I),UM(I),UN1(I)	MASP4650
6064	FORMAT(' NAMED MASS'2A4,'+'12,'DOES NOT FIT AT MASS'F8.3,'+'F6.3)	MASP4660
	GO TO 89	MASP4670
607	LIN(I)=-(1000*IC(I)+J)	MASP4680
	WIN(I)=0.	MASP4690
	AIN(I,1)=CLA(J)	MASP4700
61	CONTINUE	MASP4710
C	SINGLE AND MULTIPLY CHARGED ICNS	MASP4720
612	I=0	MASP4730
	NCL=K	MASP4740
	IF(NCL-MAXCL)6124,6124,6122	MASP4750
6122	WRITE(3,6123)NCL,MAXCL	MASP4760
6123	FORMAT('110,' CLUSTERS EXCEEDS MAXIMUM OF '15)	MASP4770
	KK=6123	MASP4780
	GO TO 89	MASP4790
6124	NNM=NEQ	MASP4800
	NN1=NNM+1	MASP4810
	K = 0	MASP4820
613	I=I+1	MASP4830
	IF(UMN(I))615,651,617	MASP4840
615	I=I+1	MASP4850
	GO TO 651	MASP4860
617	K=C	MASP4870
	NEQ=NEQ+1	MASP4880

	CIN(NEQ)=UCI(I)	MASP4890
	UM(NEQ)=UMN(I)	MASP4900
	IF(UMN(I)-UMN(I-1))6172,651,6174	MASP4910
6172	WRITE(3,6173)UMN(I)	MASP4920
6173	FORMAT(' MASS 'F8.3,' IS OUT OF ORDER')	MASP4930
	KK=6172	MASP4940
	GO TO 89	MASP4950
6174	DO 63 JC=1,LCS	MASP4960
	CALL CONC(UMN(I)*JC,UN(I)*JC,UC)	MASP4970
	IF(UC)61742,61741,61742	MASP4980
61741	GO TO(63,61744),LGO	MASP4990
61742	IF(UC*.5**((JC-1)-.1*UCI(I))63,61744,61744	MASP5000
61744	DO 62 J=1,NIT	MASP5010
	IF(JC-LC)61748,61748,61746	MASP5020
61746	IF(MS(J)-NAME)62,61748,62	MASP5030
61748	TMCOZ=TMCOZ/JC	MASP5040
6175	IF(ABS(UMN(I)-TMCOZ)-UN(I))618,62,62	MASP5050
618	ITEMP=J+1000*JC	MASP5060
	DO 6185 L=1,NNM	MASP5070
	IF(LIN(L)-ITEMP)6185,62,6185	MASP5080
6185	CONTINUE	MASP5090
	K=K+1	MASP5100
	IF(K-NC)6187,6187,643	MASP5110
6187	AIN(NEQ,K)=TAIN(J)	MASP5120
	IN(NEQ,K)=ITEMP	MASP5130
	DO 619 L=NN1,NIN	MASP5140
	IF(LIN(L)-IN(NEQ,K))619,6188,619	MASP5150
6188	WRITE(3,6189)BLANK,MS(J),UMN(I)	MASP5160
6189	FORMAT(' '2A4,'IN MORE THAN ONE EQUATION AT MASS 'F10.2)	MASP5170
	GO TO 62	MASP5180
619	CONTINUE	MASP5190
	NIN=NIN+1	MASP5200
	LIN(NIN)=IN(NEQ,K)	MASP5210
	WIN(NIN)=TMCOZ	MASP5220
62	CONTINUE	MASP5230
63	CONTINUE	MASP5240
C	SINGLE AND MULTIPLY CHARGED CLUSTERS	MASP5250
	J1=1	MASP5260
	J2=NUN	MASP5270
	JC2=3	MASP5280
	ICL=1	MASP5290
6305	DO 64 JC=1,JC2	MASP5300
	CALL CONC(UMN(I)*JC,UN(I)*JC,UC)	MASP5310
	IF(UC)6306,63055,6306	MASP5320
63055	GO TO(64,6307),LGC	MASP5330
6306	IF(UC*.5**((JC-1)-.1*UCI(I))64,6307,6307	MASP5340
6307	DO 638 J=J1,J2	MASP5350
	CLMOZ=CLM(J)/JC	MASP5360
631	IF(ABS(UMN(I)-CLMCZ)-UN(I))632,638,638	MASP5370
632	JTEMP=-(1000*JC+J)	MASP5380
	DO 633 L=1,NNM	MASP5390
	IF(LIN(L)-JTEMP)633,638,633	MASP5400
633	CONTINUE	MASP5410
	K=K+1	MASP5420
	IF(K-NC)6335,6335,643	MASP5430
6335	AIN(NEQ,K)=CLA(J)	MASP5440
	IN(NEQ,K)=JTEMP	MASP5450
	DO 634 L=NN1,NIN	MASP5460
	IF(LIN(L)-IN(NEQ,K))634,6337,634	MASP5470
6337	WRITE(3,6189)CL1(J),CL2(J),UMN(I)	MASP5480
	GO TO 638	MASP5490

634	CONTINUE	MASP5500
	NIN=NIN+1	MASP5510
	LIN(NIN)=IN(NEQ,K)	MASP5520
	WIN(NIN)=CLMOZ	MASP5530
638	CONTINUE	MASP5540
64	CONTINUE	MASP5550
	GO TO (641,651),ICL	MASP5560
641	J1=NUN+1	MASP5570
	ICL=2	MASP5580
	J2=NCL	MASP5590
	JC2=1	MASP5600
	GO TO 6305	MASP5610
643	WRITE (3,644)NC,UMN(I)	MASP5620
644	FORMAT(' POSSIBLE IONS IN EXCESS OF I3 IGNORED AT MASS F10.2)	MASP5630
	KK=653	MASP5640
651	IF(I-AMC)613,655,655	MASP5650
C	ORDER POS IONS BY WT	MASP5660
655	IF(NIN-2000)658,658,656	MASP5670
656	WRITE(3,657)NIN	MASP5680
657	FORMAT(' TOO MANY TOTAL IONS I5)	MASP5690
	KK=655	MASP5700
	GO TO 89	MASP5710
658	J1=1	MASP5720
	I1=NNAM+1	MASP5730
	DC 6626 I=I1,NIN	MASP5740
	AMIN=WIN(I)	MASP5750
	IT=I	MASP5760
	DO 661 J=I,NIN	MASP5770
	IF(WIN(J)-AMIN)66,661,659	MASP5780
659	IF(WIN(J)-AMIN-.5)661,662,662	MASP5790
66	AMIN=WIN(J)	MASP5800
	IT=J	MASP5810
661	CONTINUE	MASP5820
662	WIN(IT)=WIN(I)	MASP5830
	WIN(I)=AMIN	MASP5840
	MIN=LIN(IT)	MASP5850
	LIN(IT)=LIN(I)	MASP5860
6626	LIN(I)=MIN	MASP5870
	K1=I1	MASP5880
	K2=I1,NC	MASP5890
	K3=K1+K2	MASP5900
	DO 667 I=I1,NEQ	MASP5910
	DO 669 J=1,NC	MASP5920
	IF(IN(I,J))663,67,663	MASP5930
663	DO 668 K4=K1,K2	MASP5940
	K=K3-K4	MASP5950
	IF(IN(I,J)-LIN(K))668,664,668	MASP5960
664	IN(I,J)=K	MASP5970
	GO TO 6685	MASP5980
668	CONTINUE	MASP5990
	K1=K2+1	MASP6000
	K2=NIN	MASP6010
	K3=K1+K2	MASP6020
	GO TO 663	MASP6030
6685	K1=I1	MASP6040
	K2=MINO(NIN,K+5)	MASP6050
	K3=K1+K2	MASP6060
669	CONTINUE	MASP6070
67	CONTINUE	MASP6080
C	ORDER IONS IN EQUATIONS BY WT	MASP6090
6705	FORMAT(1X20I6)	MASP6100

671	DO 69 I=1,NEQ	MASP6110
	J1=1	MASP6120
672	IF(AIN(I,J1))674,676,674	MASP6130
674	J1=J1+1	MASP6140
	IF(J1-NC)672,672,676	MASP6150
676	JM1=J1-1	MASP6160
	JM2=J1-2	MASP6170
	IF(JM2)69,69,678	MASP6180
678	DO 686 J=1,JM2	MASP6190
	MIN=IN(I,J)	MASP6200
	M1=J	MASP6210
	JP1=J+1	MASP6220
	IGU=2	MASP6230
	DO 682 K=JP1,JM1	MASP6240
	IF(IN(I,K)-MIN)68,682,682	MASP6250
68	MIN=IN(I,K)	MASP6260
	M1=K	MASP6270
	IGO=1	MASP6280
682	CONTINUE	MASP6290
	GO TO(684,686),IGC	MASP6300
684	IN(I,M1)=IN(I,J)	MASP6310
	IN(I,J)=MIN	MASP6320
	TEMP=AIN(I,J)	MASP6330
	AIN(I,J)=AIN(I,M1)	MASP6340
	AIN(I,M1)=TEMP	MASP6350
686	CONTINUE	MASP6360
69	CONTINUE	MASP6370
C	WRITE GROSS EQUATIONS	MASP6380
	WRITE(3,1004)REPKS,LGO	MASP6390
1004	FORMAT('IGROSS EQLATIONS'20X5A4,' TYPE '11/)	MASP6400
	CALL PRINT(NEG,1,IN,LIN)	MASP6410
C	ICN ELIMINATION TESTS - MULTIPLE PEAKS	MASP6420
	I=0	MASP6430
699	I=I+1	MASP6440
	NI=0	MASP6450
70	NI=NI+1	MASP6460
	IF(AIN(I,NI+1))701,702,701	MASP6470
701	IF(NI-NC)70,702,702	MASP6480
702	NP=0	MASP6490
	NI1=NI	MASP6500
704	NP=NP+1	MASP6510
	INP=I+NP	MASP6520
	IF(AIN(INP,1))706,706,706	MASP6530
7045	IF(UM(INP)-UM(INP-1))706,706,706	MASP6540
705	IF(INP-NEQ)704,704,706	MASP6550
706	IF(NP-1)80,80,71	MASP6560
71	IF(NI-NP)715,79,72	MASP6570
715	WRITE(3,716)UM(I),NI1,NP	MASP6580
716	FORMAT(' LINE IGNORED'F12.4,', NI='I2,', NP='I2)	MASP6590
	GO TO 79	MASP6600
72	LH=1	MASP6610
	IGN=1	MASP6620
	JGC=1	MASP6630
	J=1	MASP6640
	INC=1	MASP6650
	J1=NI+1	MASP6660
725	IF(AIN(I,J1))726,74,74	MASP6670
726	CALL HYCA(I,J,LH,NP,IGN,IN,WIN,LIN)	MASP6680
	GO TO(74,747),IGO	MASP6690
74	CALL MUCH(I,J,LH,NP,IGN,IN,LIN)	MASP6700
	GO TO(745,747),IGC	MASP6710

745	GO TO (746,748,75),JGO	MASP6720
746	LH=3	MASP6730
	JGO=2	MASP6740
	J1=J-1	MASP6750
	INC=-1	MASP6760
	J=NI	MASP6770
	GO TO 725	MASP6780
747	NI1=NI1-1	MASP6790
	GO TO 75	MASP6800
748	LH=2	MASP6810
	JGO=3	MASP6820
75	J=J+INC	MASP6830
	IF(J-J1)725,76,725	MASP6840
76	IF(NI1-NP)715,79,773	MASP6850
C		MASP6860
	RESOLUTION TEST	MASP6870
773	J=0	MASP6880
7732	J=J+1	MASP6890
	INIJ=IN(I,J)	MASP6900
	IF(INIJ)7732,7732,7734	MASP6910
7734	WT=SIGN(WIN(INIJ),AIN(I,J))	MASP6920
	WT1=WT	MASP6930
	AMIN=1.	MASP6940
	JJ1=J+1	MASP6950
	DO 78 J=JJ1,NI	MASP6960
	INIJ=IN(I,J)	MASP6970
	IF(INIJ)78,78,774	MASP6980
774	WT1=SIGN(WIN(INIJ),AIN(I,J))	MASP6990
	IF(ABS(ABS(WT)-WT1)-AMIN)775,78,78	MASP7000
775	K=J	MASP7010
	AMIN=ABS(WT)-WT1	MASP7020
78	WT=WT1	MASP7030
	AIN(I,K)=-AIN(I,K)	MASP7040
	NI1=NI1-1	MASP7050
	IF(NI1-NP)79,79,773	MASP7060
79	II=I	MASP7070
	M=1	MASP7080
	I=I-1	MASP7090
	DO 798 K=1,NI	MASP7100
	IF(IN(II,K))756,798,792	MASP7110
792	IF(AIN(II,K))794,799,799	MASP7120
793	I=I+1	MASP7130
	M=0	MASP7140
794	M=M+1	MASP7150
	AIN(II,K)=ABS(AIN(II,K))	MASP7160
	IF(I-II)796,798,796	MASP7170
796	IN(I,M)=IN(II,K)	MASP7180
	AIN(I,M)=AIN(II,K)	MASP7190
	IN(II,K)=-1	MASP7200
	IAN(II,K)=ILF(0)	MASP7210
798	CONTINUE	MASP7220
799	I=II+NP-1	MASP7230
	GO TO 88	MASP7240
C		MASP7250
	SINGLE PEAK	MASP7260
80	IGO=1	MASP7270
	LH=1	MASP7280
	J1=NI+1	MASP7290
	INC=+1	MASP7300
	J=1	MASP7310
	GO TO 86	MASP7320
825	CALL FYCA(I,J,LH,NP,IGO,IN,WIN,LIN)	
	GO TO(84,85),IGO	

84	CALL MUCH(I,J,LH,NP,IGO,IN,LIN)	MASP7330
85	J=J+INC	MASP7340
	IF(J-J1)86,88,86	MASP7350
86	IF(AIN(I,J))825,85,84	MASP7360
88	IF(I-NEQ)699,90,90	MASP7370
89	WRITE(3,8989)KK	MASP7380
891	READ(1,892)IENC	MASP7390
892	FORMAT(A4)	MASP7400
	IF(IENC+975846336)851,28,851	MASP7410
8989	FORMAT(' MASP ABORT STMT 'I4)	MASP7420
C	WRITE NET EQUATIONS	MASP7430
90	WRITE(3,1005)REMK5,LGO	MASP7440
1005	FORMAT('1NET EQUATIONS'20X5A4,' TYPE 'I1/)	MASP7450
	CALL PRINT(NEQ,1,IN,LIN)	MASP7460
C	PACK EQUATIONS BEFORE SOLVING	MASP7470
	DO 923 I=1,NEQ	MASP7480
	J=0	MASP7490
	J1=0	MASP7500
92	J1=J1+1	MASP7510
920	J=J+1	MASP7520
	IF(J-NC)921,921,9225	MASP7530
921	IF(IN(I,J))92C,92C,922	MASP7540
922	AIN(I,J1)=AIN(I,J)	MASP7550
	IN(I,J1)=IN(I,J)	MASP7560
	GO TO 92	MASP7570
9225	DO 9227 J=J1,NC	MASP7580
	AIN(I,J)=0.	MASP7590
9227	IN(I,J)=0	MASP7600
923	CONTINUE	MASP7610
	DO 924 I=1,NNAM	MASP7620
	AIN(I,1)=AIN(I,1)*1000.	MASP7630
924	CIN(I)=CIN(I)*1000.	MASP7640
	DO 98 I=1,NIN	MASP7650
93	LL=LIN(I)	MASP7660
	LL2=IABS(LL)/1000	MASP7670
	LL3=IABS(LL)-LL2*1000	MASP7680
	IP1=I+1	MASP7690
	IF(LL)936,98,934	MASP7700
934	NAME1=MS(LL3)	MASP7710
	GO TO 94	MASP7720
936	NAME1=CL1(LL3)	MASP7730
	NAME2=CL2(LL3)	MASP7740
94	DO 97 J=IP1,NIN	MASP7750
	LL1=LIN(J)	MASP7760
	L22=IABS(LL1)/1000	MASP7770
	LL3=IABS(LL1)-L22*1000	MASP7780
	IF(LL*LL1)97,97,95	MASP7790
95	IF(LL)954,97,952	MASP7800
952	IF(MS(LL3)-NAME1)97,953,97	MASP7810
953	IF(LL2-L22)97,96,97	MASP7820
954	IF(CL1(LL3)-NAME1)97,956,97	MASP7830
956	IF(CL2(LL3)-NAME2)97,953,97	MASP7840
96	LIN(J)=0	MASP7850
	DO 968 K=1,NEQ	MASP7860
	DO 966 L=1,NC	MASP7870
	IF(IN(K,L)-J)966,964,966	MASP7880
964	IN(K,L)=I	MASP7890
966	CONTINUE	MASP7900
968	CONTINUE	MASP7910
97	CONTINUE	MASP7920
98	CONTINUE	MASP7930

	CALL SIMUL(AIN,IN,NEQ,CIN)	MASP7940
C	PRINT SOLVED EQUATIONS	MASP7950
	WRITE(3,1003)REMK5,LGO	MASP7960
1003	FORMAT('1 SOLVED EQUATIONS' 20X5A4,' TYPE 'I1/)	MASP7970
	CALL PRINT(NEQ,2,IN,LIN)	MASP7980
C	CALCULATE SENSITIVITIES	MASP7990
	WRITE(3,1006)REMK5,LGO	MASP8000
1006	FORMAT('1' 30X'UNIT SENSITIVITY' 20X'SENSITIVITY CORRECTION' /	MASP8010
1	50X5A4,' TYPE 'I1/6X	MASP8020
1	'ELEMENT' 10X'PPM ATOMIC' 12X'PPM WT' 12X'PPM ATOMIC' 10X'PPM WT' /)	MASP8030
1007	FORMAT(5X2A4,'+' I2,F18.5,3F20.5)	MASP8040
	IF(NSENS)984,99,984	MASP8050
984	READ(1,985) (INT1(I),UN1(I),I=1,NSENS)	MASP8060
985	FORMAT(8(A4,F6.C))	MASP8070
	DO 989 I=1,NSENS	MASP8080
	DO 987 J=1,90	MASP8090
	IF (INT1(I)-ISYM(J))987,986,987	MASP8100
986	SENS(J)=UN1(I)	MASP8110
	GO TO 989	MASP8120
987	CONTINUE	MASP8130
	WRITE(3,988)INT1(I)	MASP8140
988	FORMAT(' INVALID SENS. CHANGE' A4)	MASP8150
989	CONTINUE	MASP8160
99	DO 998 I=1,NEQ	MASP8170
	K=IN(I,1)	MASP8180
	IF(K)991,998,991	MASP8190
991	L=LIN(K)	MASP8200
	L2=IABS(L)/1000	MASP8210
	L3=IABS(L)-L2*1000	MASP8220
	IF(L)9926,9926,9928	MASP8230
9926	IEL1=CL1(L3)	MASP8240
	IEL2=CL2(L3)	MASP8250
	GO TO 9929	MASP8260
9928	IEL1=MS(L3)	MASP8270
	IEL2=BLANK	MASP8280
9929	IF(IN(I,2))993,994,993	MASP8290
993	PPMA=0.	MASP8300
	PPMW=0.	MASP8310
	SPMA=0.	MASP8320
	SPMW=0.	MASP8330
	IEL1=BLANK	MASP8340
	IEL2=BLANK	MASP8350
	L2=0	MASP8360
	GO TO 996	MASP8370
994	IF(L)995,995,9942	MASP8380
9942	DO 9944 J=1,8E	MASP8390
	IF(IEL1-ISYM(J))9944,9946,9944	MASP8400
9944	CONTINUE	MASP8410
	GO TO 9947	MASP8420
9946	PPMA=CIN(I)	MASP8430
	PPMW=PPMA*ATWT(J)/STMAS	MASP8440
	SPMA=PPMA*SS /SENS(J)	MASP8450
	SPMW=PPMW*SS /SENS(J)	MASP8460
	GO TO 996	MASP8470
C	CALC ATOMIC WT	MASP8480
9947	J=L3+1	MASP8490
	TWT=0.	MASP8500
9948	J=J-1	MASP8510
	IF(MS(J-1)-IEL1)9949,9948,9949	MASP8520
9949	TWT=TWT+TMC(J)*TAIN(J)	MASP8530
	J=J+1	MASP8540

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      IF (MS(J)-IEL1) 9955, 9949, 9955
995  J=L3+1
      TWT=0.
9951 J=J-1
      IF (CL1(J-1)-IEL1) 9953, 9952, 9953
9952 IF (CL2(J-1)-IEL2) 9953, 9951, 9953
9953 TWT=TWT+CLM(J)*CLA(J)
      J=J+1
      IF (CL1(J)-IEL1) 9955, 9954, 9955
9954 IF (CL2(J)-IEL2) 9955, 9953, 9955
9955 PPMW=CIN(I)
      PPMW=PPMA*TWT/STMAS
      SPMA=PPMA*SS
      SPMW=PPMW*SS
996  WRITE(3,1007) IEL1, IEL2, L2, PPMW, SPMA, SPMW
998  CONTINUE
      GO TO 891
1000 STOP 73
      END

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MASP8550
 MASP8560
 MASP8570
 MASP8580
 MASP8590
 MASP8600
 MASP8610
 MASP8620
 MASP8630
 MASP8640
 MASP8650
 MASP8660
 MASP8670
 MASP8680
 MASP8690
 MASP8700
 MASP8710
 MASP8720
 MASP8730

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      SUBROUTINE MUCH(I,J,LH,NP,IGC,IN,LIN)
      COMMON/TABLE/SENS(88), ATWT(88), ISYM(88), TAIN(700), TMC(700), MS(700)
      COMMON UM(300), CIN(300), CL1(400), CL2(400), CLM(400), CLA(400),
C    UN(500), UMN(500), UCI(500), LGO, BLANK, ULL, NMC, AIN(300,15)
      DIMENSION IAN(300,15)
      EQUIVALENCE (AIN(1,1), IAN(1,1))
      INTEGER*2 IN(300,15), LIN(2000)
      INTEGER CLS1, CLS2
C    MULTIPLE CHARGE TEST
      IGO=1
      L=IN(I,J)
9    LL=LIN(L)
      L2=IABS(LL/1000)
      L3=IABS(LL)-L2*1000
      Z=L2
      Y=0.
      REJ=.1
245  GO TO(25,26,28), LH
25   C=CIN(I)
      GO TO 29
26   C=CIN(I)
      DO 27 II=2,NP
      IJ=I+II-1
      IF (CIN(IJ)-C) 265, 27, 27
265  C=CIN(IJ)
27   CONTINUE
      GO TO 29
28   IJ=I+NP-1
      C=CIN(IJ)
29   IF (LL) 30, 30, 11
C    SINGLE IONS
11   L4=L3
12   L4=L4-1
      IF (MS(L4)-MS(L4+1)) 13, 12, 13
13   L5=L4
135  Y=Y+1.
      IF (Y-Z) 138, 138, 6
138  L4=L5
14   L4=L4+1
      IF (MS(L4)-MS(L3)) 135, 16, 135

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MUCH 10
 MUCH 20
 MUCH 30
 MUCH 40
 MUCH 50
 MUCH 60
 MUCH 70
 MUCH 80
 MUCH 90
 MUCH 100
 MUCH 110
 MUCH 120
 MUCH 130
 MUCH 140
 MUCH 150
 MUCH 160
 MUCH 170
 MUCH 180
 MUCH 190
 MUCH 200
 MUCH 210
 MUCH 220
 MUCH 230
 MUCH 240
 MUCH 250
 MUCH 260
 MUCH 270
 MUCH 280
 MUCH 290
 MUCH 300
 MUCH 310
 MUCH 320
 MUCH 330
 MUCH 340
 MUCH 350
 MUCH 360
 MUCH 370
 MUCH 380
 MUCH 390
 MUCH 400

16	IF (ABS(TAIN(L4))- .05*ABS(TAIN(L3)))135,18,18	MUCH 410
18	AIR=TAIN(L3)/TAIN(L4)	MUCH 420
20	AMN =TMC(L4)/Y	MUCH 430
	CALL CONC(AMN,0 ,UC)	MUCH 440
	IF(UC)24,22,24	MUCH 450
22	GO TO(23,14),LGO	MUCH 460
23	UC=UL1*SQR(TAMN)**3	MUCH 470
24	IF(.5**(Z-Y)*AIR*UC -REJ*C 146,14,14	MUCH 480
C	CLUSTERS	MUCH 490
30	L4=L3	MUCH 500
32	L4=L4-1	MUCH 510
	IF(CL1(L4)-CL1(L4+1))335,33,335	MUCH 520
33	IF(CL2(L4)-CL2(L4+1))335,32,335	MUCH 530
335	L5=L4	MUCH 540
336	Y=Y+1.	MUCH 550
	IF(Y-Z)338,338,6	MUCH 560
338	L4=L5	MUCH 570
34	L4=L4+1	MUCH 580
	IF(CL1(L4)-CL1(L3))336,35,336	MUCH 590
35	IF(CL2(L4)-CL2(L3))336,36,336	MUCH 600
36	IF(ABS(CLA(L4))- .2*ABS(CLA(L3)))336,38,38	MUCH 610
38	AIR=CLA(L3)/CLA(L4)	MUCH 620
40	AMN=CLM(L4)/Y	MUCH 630
	CALL CONC(AMN,0 ,UC)	MUCH 640
	IF(UC)44,42,44	MUCH 650
42	GO TO(43,34),LGO	MUCH 660
43	UC=UL1	MUCH 670
44	IF(.2**(Z-Y)*AIR*UC -REJ*C 146,34,34	MUCH 680
46	L6=Y	MUCH 690
	IGO=2	MUCH 700
	IAN(I,J)=ILF((L4-L5)*100+L6)	MUCH 710
	IN(I,J)=-IN(I,J)	MUCH 720
6	RETURN	MUCH 730
	END	MUCH 740
	SUBROUTINE HYCA(I,J,LH,NP,IGO,IN,WIN,LIN)	HYCA 10
C	HYDROCARBON TEST	HYCA 20
	COMMON UM(300),CIN(300),CL1(400),CL2(400),CLM(400),CLA(400),	HYCA 30
C	UN(500),UMN(500),UCI(500),LGC,BLANK,UL1,NMC,AIN(300,15)	HYCA 40
	DIMENSION WIN(2000)	HYCA 50
	DIMENSION IAN(300,15)	HYCA 60
	EQUIVALENCE (AIN(1,1),IAN(1,1))	HYCA 70
	INTEGER*2 IN(300,15),LIN(2000)	HYCA 80
	AIN(I,J)=ABS(AIN(I,J))	HYCA 90
	K=IN(I,J)	HYCA 100
	IC=IABS(LIN(K)/1000)	HYCA 110
	WT=WIN(K)*IC-1.007825	HYCA 120
	GO TO(25,26,28),LH	HYCA 130
25	C=CIN(I)	HYCA 140
	GO TO 29	HYCA 150
26	C=CIN(I)	HYCA 160
	DO 27 II=2,NP	HYCA 170
	IJ=I+II-1	HYCA 180
	IF(CIN(IJ)-C)265,27,27	HYCA 190
265	C=CIN(IJ)	HYCA 200
27	CONTINUE	HYCA 210
	GO TO 29	HYCA 220
28	IJ=I+NP-1	HYCA 230
	C=CIN(IJ)	HYCA 240
29	DO 40 L=1, IC	HYCA 250

	W=WT/L	HYCA 260
	CALL CONC(W,0,UC)	HYCA 270
	IF(UC)22,10,22	HYCA 280
10	GO TO(12,40),LGO	HYCA 290
12	UC=UL1	HYCA 300
22	IF(UC-.1*C*5.**((IC-L))34,34,40	HYCA 310
34	IAN(I,J)=ILF(L)	HYCA 320
	IN(I,J)=-IN(I,J)	HYCA 330
	IGO=2	HYCA 340
	RETURN	HYCA 350
40	CONTINUE	HYCA 360
	IGG=1	HYCA 370
	RETURN	HYCA 380
	END	HYCA 390
	SUBROUTINE CONC(W,UNC,UC)	CONC 10
	COMMON UM(300),CIN(300),CL1(400),CL2(400),CLM(400),CLA(400),	CONC 20
	C UN(500),UMN(500),UCI(500),LGO,BLANK,UL1,NMC	CCNC 30
	M=0	CONC 40
1	M=M+1	CCNC 50
	IF(UNC-UN(M))3,2,2	CCNC 60
2	UNCM=UNC	CCNC 70
	GO TO 4	CONC 80
3	UNCM=UN(M)	CONC 90
4	IF(UMN(M))34,6,6	CONC 100
6	IF(UMN(M)-W+UNCM)38,8,8	CCNC 110
8	IF(UMN(M)-W-UNCM)14,14,10	CONC 120
10	UC=0.	CONC 130
	GO TO 22	CONC 140
14	UC=UCI(M)	CONC 150
25	IF(UMN(M)-UMN(M+1))22,26,22	CCNC 160
26	M=M+1	CONC 170
	IF(UCI(M)-UC)25,25,28	CCNC 180
28	UC=UCI(M)	CCNC 190
	GO TO 25	CONC 200
22	CONTINUE	CCNC 210
	RETURN	CONC 220
	NEGATIVE INFO REGION	CCNC 230
34	IF(-UMN(M)-W-UNCM)36,10,10	CCNC 240
36	IF(-UMN(M+1)-W+UNCM)37,28,28	CONC 250
37	M=M+1	CONC 260
38	IF(M-NMC)1,10,10	CCNC 270
	END	CONC 280
	SUBROUTINE SIMUL(A,M,NE,V)	SIML 10
C	A IS BANDEC MATRIX,M IS SUBSCRIPT MATRIX FOR A	SIML 20
C	NE IS NUMBER OF EQUATIONS,V IS VECTOR	SIML 30
	DIMENSION A(300,15),M(300,15),T(20),V(500),MT(20)	SIML 40
	INTEGER*2 M	SIML 50
C	SEQUENCE EACH ROW	SIML 60
101	FORMAT(20I5)	SIML 70
	NC=15	SIML 80
	DO 15 I=1,NE	SIML 90
	J1=1	SIML 100
2	IF(A(I,J1))3,4,3	SIML 110
3	J1=J1+1	SIML 120
	GO TO 2	SIML 130
4	JM1=J1-1	SIML 140
	JM2=J1-2	SIML 150

	IF(JM2)15,15,5	SIML 160
5	DC 10 J=1,JM2	SIML 170
	MIN=M(I,J)	SIML 180
	M1=J	SIML 190
	JP1=J+1	SIML 200
	IGO=2	SIML 210
	DC 7 K=JP1,JM1	SIML 220
	IF(M(I,K)-MIN)6,7,7	SIML 230
6	MIN=M(I,K)	SIML 240
	M1=K	SIML 250
	IGO=1	SIML 260
7	CONTINUE	SIML 270
	GO TO(8,10),IGO	SIML 280
8	M(I,M1)=M(I,J)	SIML 290
	M(I,J)=MIN	SIML 300
	TEMP=A(I,J)	SIML 310
	A(I,J)=A(I,M1)	SIML 320
	A(I,M1)=TEMP	SIML 330
10	CONTINUE	SIML 340
15	CONTINUE	SIML 350
C	START FORWARD SOLUTION	SIML 360
C	FIND MIN M WITH LARGEST A IN FIRST COL	SIML 370
	NEM1=NE-1	SIML 380
	DO 60 I=1,NEM1	SIML 390
	IP1=I+1	SIML 400
	MIN=100000	SIML 410
	DO 30 J=I,NE	SIML 420
	IF(M(J,1)-MIN)24,16,30	SIML 430
16	IF(ABS(A(J,1))-AMAX)20,21,17	SIML 440
17	IF(ABS(A(J,1))-AMAX*5.)18,26,26	SIML 450
18	IF(A(J,2))19,26,19	SIML 460
19	IF(A(M1,2))26,30,26	SIML 470
20	IF(ABS(A(J,1))*5.-AMAX)30,21,21	SIML 480
21	IF(A(J,2))30,22,30	SIML 490
22	IF(A(M1,2))26,30,26	SIML 500
24	IF(M(J,1))30,30,25	SIML 510
25	MIN=M(J,1)	SIML 520
26	M1=J	SIML 530
	AMAX=ABS(A(J,1))	SIML 540
30	CONTINUE	SIML 550
	IF(MIN-100000)31,60,60	SIML 560
31	IF(M1-I)35,35,37	SIML 570
32	DO 34 K=1,NC	SIML 580
	TEMP=M(I,K)	SIML 590
	M(I,K)=M(M1,K)	SIML 600
	M(M1,K)=TEMP	SIML 610
	TEMP=A(I,K)	SIML 620
	A(I,K)=A(M1,K)	SIML 630
34	A(M1,K)=TEMP	SIML 640
	TEMP=V(I)	SIML 650
	V(I)=V(M1)	SIML 660
	V(M1)=TEMP	SIML 670
C	IF FIRST ELEMENT IN OTHER ROWS,PURGE	SIML 680
35	DO 58 J=IP1,NE	SIML 690
	IF(M(J,1)-M(I,1))58,36,58	SIML 700
36	RAT=-A(J,1)/A(I,1)	SIML 710
	V(J)=V(J)+V(I)*RAT	SIML 720
	L1=2	SIML 730
	L2=2	SIML 740
	L=0	SIML 750
37	IF(M(I,L1)-M(J,L2))38,46,42	SIML 760

38	IF(M(I,L1))44,44,40	SIML 770
40	L=L+1	SIML 780
	T(L)=A(I,L1)*RAT	SIML 790
	MT(L)=M(I,L1)	SIML 800
	L1=L1+1	SIML 810
	GO TO 49	SIML 820
42	IF(M(J,L2))40,40,44	SIML 830
44	L=L+1	SIML 840
	T(L)=A(J,L2)	SIML 850
	MT(L)=M(J,L2)	SIML 860
	L2=L2+1	SIML 870
	GO TO 49	SIML 880
46	IF(M(I,L1))54,54,48	SIML 890
48	L=L+1	SIML 900
	T(L)=A(J,L2)+A(I,L1)*RAT	SIML 910
	MT(L)=M(I,L1)	SIML 920
	L1=L1+1	SIML 930
	L2=L2+1	SIML 940
	IF(T(L))49,485,49	SIML 950
485	L=L-1	SIML 960
49	IF(L-NC)37,50,50	SIML 970
50	WRITE(3,51)I,J,L,((M(N1,M1),M1=1,NC),N1=1,NE)	SIML 980
51	FORMAT(6H1ABORT3110/(1015))	SIML 990
54	IF(L)561,561,55	SIML1000
55	DO 56 LL=1,L	SIML1010
	M(J,LL)=MT(LL)	SIML1020
56	A(J,LL)=T(LL)	SIML1030
561	LP1=L+1	SIML1040
	DO 57 LL=LP1,NC	SIML1050
	M(J,LL)=0	SIML1060
57	A(J,LL)=0.	SIML1070
58	CONTINUE	SIML1080
100	FORMAT(2I10)	SIML1090
1	FORMAT(1XF7.2,F7.2,I4,F7.2,I4,F7.2,I4,F7.2,I4,F7.2,I4,F7.2,I4,	SIML1100
	1 F7.2,I4,F7.2,I4,F7.2,I4,F7.2,I4)	SIML1110
60	CONTINUE	SIML1120
C	BACKWARD SOLUTION	SIML1130
	DO 98 II=2,NE	SIML1140
	I= NE+2-II	SIML1150
	IM1=I-1	SIML1160
	DO 62 J=1,NC	SIML1170
	J1=J-1	SIML1180
	IF(M(I,J))64,64,62	SIML1190
62	CONTINUE	SIML1200
64	IF(J1)98,98,65	SIML1210
65	DO 90 J=1,IM1	SIML1220
	DC 66 K=1,NC	SIML1230
	K1=K-1	SIML1240
	IF(M(J,K))68,68,66	SIML1250
66	CONTINUE	SIML1260
68	IF(K1)90,90,70	SIML1270
C	IF LAST ELEMENT IN OTHER ROWS,PURGE	SIML1280
70	DO 71 K2=2,K	SIML1290
	IF(M(I,J1)-M(J,K2))71,72,71	SIML1300
71	CONTINUE	SIML1310
	GO TO 90	SIML1320
72	RAT=-A(J,K2)/A(I,J1)	SIML1330
	V(J)=V(J)+V(I)*RAT	SIML1340
	L1=1	SIML1350
	L2=1	SIML1360
	L=0	SIML1370

74	IF(L1-J1)77,75,75	SIML1380
75	IF(L2-K2)76,755,76	SIML1390
755	L2=L2+1	SIML1400
76	IF(L2-K1)80,80,86	SIML1410
77	IF(M(I,L1)-M(J,L2))78,82,80	SIML1420
78	L=L+1	SIML1430
	T(L)=A(I,L1)*RAT	SIML1440
	MT(L)=M(I,L1)	SIML1450
	L1=L1+1	SIML1460
	GO TO 74	SIML1470
80	L=L+1	SIML1480
	T(L)=A(J,L2)	SIML1490
	MT(L)=M(J,L2)	SIML1500
81	L2=L2+1	SIML1510
	GO TO 74	SIML1520
82	L=L+1	SIML1530
	T(L)=A(I,L1)*RAT+A(J,L2)	SIML1540
	MT(L)=M(I,L1)	SIML1550
	L1=L1+1	SIML1560
	L2=L2+1	SIML1570
	IF(T(L))74,84,74	SIML1580
84	L=L-1	SIML1590
	GO TO 74	SIML1600
86	IF(L)89,89,87	SIML1610
87	UL 88 LL=1,L	SIML1620
	A(J,LL)=T(LL)	SIML1630
88	M(J,LL)=MT(LL)	SIML1640
89	LP1=L+1	SIML1650
	DO 895 LL=LP1,NC	SIML1660
	A(J,LL)=0.	SIML1670
895	M(J,LL)=0	SIML1680
90	CONTINUE	SIML1690
98	CONTINUE	SIML1700
	DO 99 I=1,NE	SIML1710
	IF(A(I,1))985,99,985	SIML1720
985	V(I)=V(I)/A(I,1)	SIML1730
	DO 986 J=2,NC	SIML1740
	IF(A(I,J))986,989,986	SIML1750
986	A(I,J)=A(I,J)/A(I,1)	SIML1760
989	A(I,1)=1.	SIML1770
99	CONTINUE	SIML1780
	RETURN	SIML1790
	END	SIML1800
	SLBRoutine PRINT(NEQ,LL,IA,LIN)	PRNT 10
	COMMON/TABLE/SENS(88),ATWT(88),ISYM(88),TAIN(700),TMC(700),MS(700)	PRNT 20
	COMMON UM(300),CIN(300),CL1(400),CL2(400),CLM(400),CLA(400),	PRNT 30
C	UN(500),UMN(500),UCI(500),LGO,BLANK,UL1,NMC,AIN(300,15)	PRNT 40
	DIMENSION MCG(20),NAM1(20),NAM2(20)	PRNT 50
	DIMENSION IAN(300,15)	PRNT 60
	EQUIVALENCE (AIN(1,1),IAN(1,1))	PRNT 70
	INTEGER*2 IN(300,15),LIN(2000)	PRNT 80
	INTEGER BLANK,CL1,CL2	PRNT 90
	NC=15	PRNT 100
	WT=0.	PRNT 110
	DO 919 I=1,NEQ	PRNT 120
	J=0	PRNT 130
	GO TO 913	PRNT 140
909	J=J+1	PRNT 150
91	K=IN(I,J)	PRNT 160

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          IF(LIN(K)) 912,912,911          PRNT 170
910      J=J+1                            PRNT 180
          MCG(J)=0                        PRNT 190
          NAM1(J)=BLANK                   PRNT 200
          NAM2(J)=IAN(I,J)                PRNT 210
          GO TO 9125                       PRNT 220
911      MCG(J)=LIN(K)/1000               PRNT 230
          L=LIN(K)-MCG(J)*1000            PRNT 240
          NAM1(J)=BLANK                   PRNT 250
          NAM2(J)=MS(L)                   PRNT 260
          GO TO 9125                       PRNT 270
912      MCG(J)=-LIN(K)/1000              PRNT 280
          L=-LIN(K)-MCG(J)*1000           PRNT 290
          NAM1(J)=CL1(L)                   PRNT 300
          NAM2(J)=CL2(L)                   PRNT 310
9125     IF(J-NC)913,914,914              PRNT 320
913      IF(IN(I,J+1))910,914,909         PRNT 330
914      IF(J)915,915,916                 PRNT 340
915      J=1                              PRNT 350
          NAM1(1)=BLANK                   PRNT 360
          NAM2(1)=BLANK                   PRNT 370
          MCG(1)=0                         PRNT 380
916      NJ=J                             PRNT 390
          GO TO(917,918),LL               PRNT 400
917      WT=UM(I)                         PRNT 410
918      WRITE(3,1004)WT,CIN(I),(AIN(I,J),NAM1(J),NAM2(J),MCG(J),J=1,NJ) PRNT 420
1004     FORMAT(F8.3,F12.4,'='F7.4,2A4,'+'I2,4('+'F7.4,2A4,'+'I2) PRNT 430
          /5('+'F7.4,2A4,'+'I2))          PRNT 440
919      CONTINUE                         PRNT 450
          RETURN                           PRNT 460
          END                             PRNT 470

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          BLOCK DATA                     TABL 10
          COMMON/TABLE/SENS(88),ATWT(88),ISYM(88),TAIN(700),TMC(700),MS(700) TABL 20
          DIMENSION TMC1(133),TMC2(25),TAIN1(133),TAIN2(25) TABL 30
          EQUIVALENCE(TMC(267),TMC1(134),TMC2(1)),(TAIN(267),TAIN1(134), TABL 40
          E                                TAIN2(1)) TABL 50
          DATA SENS/                     TABL 50
C      H 1 HE 2 LI 3 RE 4 R 5 C 6 N 7 TABL 70
S 1.40 ,1. ,4.15 ,.614 ,.60 ,.60 ,.459 , TABL 80
C      O 8 F 9 NE 10 NA 11 MG 12 AL 13 SI 14 TABL 90
S .428 ,1.8 ,1. ,10.3 ,2.8 ,1.9 ,1.07 , TABL 100
C      P 15 S 16 CL 17 A 18 K 19 CA 20 SC 21 TABL 110
S 1.3 ,1.09 ,.80 ,1. ,18.1 ,5.6 ,.33 , TABL 120
C      TI 22 V 23 CR 24 MN 25 FE 26 CO 27 NI 28 TABL 130
S 1.31 ,1.05 ,1.3 ,2.0 ,1.00 ,.85 ,1.05 , TABL 140
C      CU 29 ZN 30 GA 31 GE 32 AS 33 SE 34 BR 35 TABL 150
S 1.75 ,3.0 ,2.19 ,2.7 ,3.5 ,2.5 ,8.3 , TABL 160
C      KR 36 RB 37 SR 38 Y 39 ZR 40 NB 41 MO 42 TABL 170
S 1. ,30.2 ,9.1 ,2.17 ,1.36 ,.782 ,.811 , TABL 180
C      RU 43 RH 44 PD 45 AG 46 CC 47 IN 48 SN 49 TABL 190
S .711 ,.01 ,1.2 ,1.91 ,4.57 ,3.70 ,2.2 , TABL 200
C      SB 50 TE 51 I 52 XE 53 CS 54 HA 55 LA 56 TABL 210
S 2.11 ,2.44 ,6.35 ,1. ,9.05 ,9.97 ,3.23 , TABL 220
C      CE 57 PR 58 ND 59 SM 60 EU 61 GD 62 TR 63 TABL 230
S 2.69 ,2.55 ,2.75 ,2.97 ,3.85 ,2.70 ,2.40 , TABL 240
C      DY 64 HO 65 ER 66 TM 67 YB 68 LU 69 HF 70 TABL 250
S 2.15 ,2.40 ,2.43 ,2.44 ,2.97 ,3.10 ,2.35 , TABL 260
C      TA 71 W 72 RE 73 OS 74 IR 75 PT 76 AU 77 TABL 270
S .55 ,.45 ,.610 ,.586 ,.580 ,.4 ,1.32 , TABL 280

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C		HG 78	TL 79	PB 80	EI 81	RA 82	TH 83	PA 84	TABL 290
S		7.60	4.90	3.82	3.23	1.	2.	1.	TABL 300
C		U 85	NP 86	PU 87	H2 88				TABL 310
S		1.	1.	1.	1.	/			TABL 320
		DATA ISYM/							TABL 330
C		1	2	3	4	5	6	7	TABL 340
I		'H'	'HE'	'LI'	'BE'	'B'	'C'	'N'	TABL 350
C		9	10	11	12	13	14	15	TABL 360
I		'F'	'NE'	'NA'	'MG'	'AL'	'SI'	'P'	TABL 370
C		17	18	19	20	21	22	23	TABL 380
I		'CL'	'AR'	'K'	'CA'	'SC'	'TI'	'V'	TABL 390
C		25	26	27	28	29	30	31	TABL 400
I		'MN'	'FE'	'CO'	'NI'	'CU'	'ZN'	'GA'	TABL 410
C		33	34	35	36	37	38	39	TABL 420
I		'AS'	'SE'	'BR'	'KR'	'RR'	'SR'	'Y'	TABL 430
C		41	42	43	44	45	46	47	TABL 440
I		'NB'	'MC'	'RU'	'RH'	'PD'	'AG'	'CD'	TABL 450
C		49	50	51	52	53	54	55	TABL 460
I		'SN'	'SB'	'TE'	'I'	'XE'	'CS'	'BA'	TABL 470
C		57	58	59	60	61	62	63	TABL 480
I		'CE'	'FR'	'ND'	'SM'	'EU'	'GD'	'TB'	TABL 490
C		65	66	67	68	69	70	71	TABL 500
I		'HC'	'ER'	'TM'	'YB'	'LU'	'HF'	'TA'	TABL 510
C		73	74	75	76	77	78	79	TABL 520
I		'RE'	'GS'	'IR'	'PT'	'AU'	'HG'	'TL'	TABL 530
C		81	82	83	84	85	86	87	TABL 540
I		'BI'	'RA'	'TH'	'PA'	'U'	'NP'	'PU'	TABL 550
		DATA ATWT/							TABL 560
C		H 1	HE 2	LI 3	RE 4	R 5	C 6	N 7	TABL 570
W		1.00797	4.0026	6.939	5.0122	10.811	12.0115	14.007	TABL 580
C		O 8	F 9	NE 10	NA 11	MG 12	AL 13	SI 14	TABL 590
W		15.9994	18.9984	20.183	22.9898	24.312	26.9815	28.086	TABL 600
C		P 15	S 16	CL 17	A 18	K 19	CA 20	SC 21	TABL 610
W		30.9738	28.086	35.453	35.948	39.102	40.08	44.956	TABL 620
C		TI 22	V 23	CR 24	MN 25	FE 26	CO 27	NI 28	TABL 630
W		47.90	50.942	51.996	54.938	55.847	58.933	58.71	TABL 640
C		CU 29	ZN 30	GA 31	GE 32	AS 33	SE 34	RR 35	TABL 650
W		63.54	65.37	69.72	72.55	74.922	78.96	79.909	TABL 660
C		KR 36	RB 37	SR 38	Y 39	ZR 40	NB 41	MC 42	TABL 670
W		83.80	85.47	87.62	88.905	91.22	92.906	95.54	TABL 680
C		KU 43	RH 44	PD 45	AG 46	CD 47	IN 48	SN 49	TABL 690
W		101.11	102.91	106.4	107.87	112.40	114.82	118.69	TABL 700
C		3B 50	TE 51	I 52	XE 53	CS 54	RA 55	LA 56	TABL 710
W		121.75	127.60	126.90	131.30	132.91	137.34	138.91	TABL 720
C		CE 57	PR 58	ND 59	SM 60	EU 61	GD 62	TB 63	TABL 730
W		140.12	140.91	144.24	150.35	151.96	157.25	158.92	TABL 740
C		DY 64	HO 65	ER 66	TM 67	YB 68	LU 69	HF 70	TABL 750
W		162.50	164.93	167.26	168.93	173.04	174.97	178.49	TABL 760
C		TA 71	W 72	RE 73	CS 74	IR 75	PT 76	AU 77	TABL 770
W		180.55	183.85	186.2	190.2	192.2	195.09	196.97	TABL 780
C		HG 78	TL 79	PB 80	EI 81	RA 82	TH 83	PA 84	TABL 790
W		200.59	204.37	207.19	208.98	226.	232.05	231.	TABL 800
C		U 85	NP 86	PU 87	H2 88				TABL 810
W		228.67	237.	242.	240.1594	/			TABL 820
		DATA TAIN/							TABL 830
C		H 1	H2 2	HE 3	LI 5		6	BE 7	TABL 840
A		-100.	-100.	99.99986	100.000137	92.58	7.42	100.	TABL 850
C		B 8		C 10	11	N 12	13	O 14	TABL 860
A		80.29	19.61	98.893	1.107	99.6327	3.663	95.759	TABL 870
C		15	16	F 17	NE 18	19	20	NA 21	TABL 880
A		.2039	.0374	100.	90.92	8.82	.257	100.	TABL 890

C	MG 22	23	24	AL 25	SI 26	27	28	TABL 900
A	78.70	,11.17	,10.13	,100.	,52.21	,4.70	,3.09	, TABL 910
C	P 29	S 30	31	32	33	CL 34	35	TABL 920
A	100.	,95.0	,4.22	,.76C	,.0136	,75.529	,24.471	, TABL 930
C	AR 36	37	38	K 39	40	41	CA 42	TABL 940
A	59.60	,.337	,.063	,93.1	,6.88	,.01181	,96.97	, TABL 950
C	43	44	45	46	47	SC 48	TI 49	TABL 960
A	2.06	,.64	,.185	,.146	,.0033	,100.	,73.98	, TABL 970
C	50	51	52	53	V 54	55	CR 56	TABL 980
A	8.0	,7.29	,5.51	,5.34	,99.76	,.24	,83.76	, TABL 990
C	57	58	59	MA 60	FE 61	62	63	TABL1000
A	9.55	,4.31	,2.38	,100.	,91.66	,5.82	,2.19	, TABL1010
C	64	CO 65	NI 66	67	68	69	70	TABL1020
A	.33	,100.	,67.88	,26.23	,3.66	,1.19	,1.08	, TABL1030
C	CU 71	72	ZN 73	74	75	76	77	TABL1040
A	69.09	,30.91	,48.89	,27.81	,18.57	,4.11	,.62	, TABL1050
C	GA 78	79	GE 80	81	82	83	84	TABL1060
A	60.4	,39.6	,36.54	,27.43	,20.52	,7.76	,7.76	, TABL1070
C	AS 85	SE 86	87	88	89	90	91	TABL1080
A	100.	,49.82	,23.52	,9.19	,9.02	,7.58	,.87	, TABL1090
C	BR 92	93	KR 94	95	96	97	98	TABL1100
A	50.537	,49.463	,56.9	,17.37	,11.56	,11.55	,2.27	, TABL1110
C	99	RB 100	101	SR 102	103	104	105	TABL1120
A	.354	,72.15	,27.85	,82.56	,9.86	,7.02	,.56	, TABL1130
C	Y 106	ZR 107	108	109	110	111	NE 112	TABL1140
A	100.	,51.46	,17.4	,17.11	,11.22	,2.8	,100.	, TABL1150
C	MO 113	114	115	116	117	118	119	TABL1160
A	23.78	,16.53	,15.84	,15.72	,9.63	,9.46	,9.04	, TABL1170
C	RU 120	121	122	123	124	125	126	TABL1180
A	31.61	,18.58	,17.07	,12.72	,12.62	,5.51	,1.87	, TABL1190
C	RH 127	PD 128	129	130	131	132	133	TABL1200
A	100.	,27.33	,26.71	,22.23	,11.81	,10.97	,.96	/ TABL1210
	DATA TAIN1/							TABL1220
C	AG 134	135	CD 136	137	138	139	140	TABL1230
A	51.35	,48.65	,28.86	,24.07	,12.75	,12.39	,12.26	, TABL1240
C	141	142	143	IN 144	145	SN 146	147	TABL1250
A	7.58	,1.215	,.875	,95.72	,4.28	,32.85	,24.03	, TABL1260
C	148	149	150	151	152	153	154	TABL1270
A	14.3	,8.58	,7.61	,5.94	,4.72	,.96	,.66	, TABL1280
C	155	SB 156	157	TE 158	159	160	161	TABL1290
A	.35	,57.25	,42.75	,34.48	,31.79	,18.71	,6.99	, TABL1300
C	162	163	164	165	I 166	XE 167	168	TABL1310
A	4.61	,2.46	,.87	,.C89	,100.	,26.89	,26.44	, TABL1320
C	169	170	171	172	173	174	175	TABL1330
A	21.18	,10.44	,8.87	,4.08	,1.919	,1.09	,.C096	, TABL1340
C	CS 176	BA 177	178	179	180	181	182	TABL1350
A	100.	,71.66	,11.32	,7.81	,6.59	,2.42	,.101	, TABL1360
C	183	LA 184	185	CE 186	187	188	189	TABL1370
A	.097	,99.911	,.089	,88.48	,11.07	,.25	,.193	, TABL1380
C	PR 190	ND 191	192	193				

C		232	233	234	235	236	LU 237	238	TABL1510
A	16.13	,14.31	,12.73	,3.03	,.135	,57.41	,2.59	,	TABL1520
C	HF 239	240	241	242	243	244	TA 245	,	TABL1530
A	35.24	,27.14	,18.5	,13.75	,5.2	,.18	,99.9877	,	TABL1540
C	246	W 247	248	249	250	251	RE 252	,	TABL1550
A	.0123	,30.64	,28.41	,26.41	,14.4	,.135	,62.93	,	TABL1560
C	253	US 254	255	256	257	258	259	,	TABL1570
A	37.07	,41.0	,26.4	,16.1	,13.3	,1.64	,1.59	,	TABL1580
C	260	IR 261	262	PT 263	264	265	266	,	TABL1590
A	.018	,62.7	,37.3	,33.8	,32.9	,25.3	,7.21	/	TABL1600
	DATA TAIN2/								TABL1610
C	267	268	AU 269	HG 270	271	272	273	,	TABL1620
A	.78	,.0127	,100.	,25.8	,23.13	,16.84	,13.22	,	TABL1630
C	274	275	276	TL 277	278	PA 279	280	,	TABL1640
A	10.02	,6.85	,.146	,70.5	,29.5	,52.3	,23.6	,	TABL1650
C	281	282	RI 283	RA 284	TH 285	PA 286	U 287	,	TABL1660
A	22.6	,1.48	,100.	,100.	,100.	,100.	,99.2739	,	TABL1670
C	288	289	NP 290	PU 291				,	TABL1680
A	.7204	,.0056	,100.	,100.	/			,	TABL1690
	DATA TMC/								TABL1700
C	F	1	H2	2	HE	3	4	L1	5
M	1.007825	,2.015650	,4.002601	,3.016027	,7.016001	,6.015121	,9.012154	,	TABL1710
C	8	9	C	10	11	N	12	13	O
M	11.00931	,10.01294	,12.	,13.00336	,14.00307	,15.00011	,15.99491	,	TABL1720
C	15	16	F	17	NE	18	19	20	NA
M	17.99916	,16.99913	,18.99840	,19.99244	,21.99138	,20.99385	,22.98978	,	TABL1730
C	MG	22	23	24	AL	25	SI	26	27
M	23.98504	,25.98259	,24.98584	,26.98154	,27.97693	,28.97649	,29.97376	,	TABL1740
C	P	29	S	30	31	32	33	CL	34
M	30.97376	,31.97207	,33.96786	,32.97146	,35.96709	,34.96885	,36.96590	,	TABL1750
C	AR	36	37	38	K	39	40	41	CA
M	39.96239	,35.96755	,37.96273	,38.96371	,40.96183	,39.96400	,39.96259	,	TABL1760
C	43	44	45	46	47	SC	48	TI	49
M	43.95546	,41.95863	,47.95253	,42.95878	,45.95369	,44.95592	,47.94795	,	TABL1770
C	50	51	52	53	V	54	55	CR	56
M	45.95263	,46.95176	,48.94787	,49.94479	,50.94398	,49.94716	,51.94051	,	TABL1780
C	57	58	59	MN	60	FE	61	62	63
M	52.94065	,49.94605	,53.93887	,54.93805	,55.93494	,53.93961	,56.93541	,	TABL1790
C	64	CC	65	NI	66	67	68	69	70
M	57.93331	,58.93318	,57.93335	,59.93077	,61.92834	,60.93109	,63.92756	,	TABL1800
C	CU	71	72	ZN	73	74	75	76	77
M	62.92959	,64.92778	,63.92914	,65.92605	,67.92486	,66.92714	,69.92534	,	TABL1810
C	GA	78	79	GE	80	81	82	83	84
M	68.92571	,70.92482	,73.92100	,71.92159	,69.92399	,72.92334	,75.92129	,	TABL1820
C	AS	85	SE	86	87	88	89	90	91
M	74.92171	,79.91647	,77.91739	,81.91663	,75.91928	,76.91998	,73.92254	,	TABL1830
C	BR	92	93	KR	94	95	96	97	98
M	78.91839	,80.91642	,83.91151	,85.91079	,81.91345	,82.91405	,79.91659	,	TABL1840
C	99	RB	100	101	SR	102	103	104	105
M	77.92019	,84.91202	,86.90930	,87.90601	,85.90935	,86.90899	,83.91325	,	TABL1850
C	Y	106	ZR	107	108	109	110	111	NE
M	88.90572	,89.90433	,93.90764	,91.90467	,90.90532	,95.90930	,92.90566	,	TABL1860
C	MO	113	114	115	116	117	118	119	
M	97.90598	,95.90496	,91.90855	,94.90444	,99.90651	,96.90621	,93.90594	,	TABL1870
C	RU	120	121	122	123	124	125	126	
M	101.9037	,103.9042	,100.9050	,98.90605	,99.90500	,95.90870	,97.95400	,	TABL1880
C	RH	127	PD	128	129	130	131	132	133
M	102.9046	,105.9029	,107.9035	,104.9048	,109.9045	,103.9033	,101.9049	,	TABL1890
	DATA TMC1/								TABL1900
C	AG	134	135	CD	136	137	138	139	140
M	106.9048	,108.9046	,113.9036	,111.9031	,110.9043	,109.9033	,112.9045	,	TABL1910

C		141	142	143	IN 144	145	SN 146	147	TABL2120		
M	115.9050,105.9059,107.9041,114.9036,112.9043,119.9022,117.9020,								TABL2130		
C		148	149	150	151	152	153	154	TABL2140		
M	115.9022,118.9032,116.9031,123.9052,121.9035,111.9051,113.9039,								TABL2150		
C		155	SE 156	157	TE 158	159	160	161	TABL2160		
M	114.9034,120.9037,122.9042,129.9070,127.9056,125.9039,124.9046,								TABL2170		
C		162	163	164	165	I 166	XE 167	168	TABL2180		
M	123.9031,121.9029,122.9043,119.9045,126.9047,131.9042,128.9047,								TABL2190		
C		169	170	171	172	173	174	175	TABL2200		
M	130.9051,133.9054,135.9072,129.9035,127.9035,125.9045,123.9061,								TABL2210		
C		CS 176	BA 177	178	179	180	181	182	TABL2220		
M	132.9051,137.9049,136.9056,135.9044,134.9056,133.9043,129.9062,								TABL2230		
C		183	LA 184	185	CE 186	187	188	189	TABL2240		
M	131.9051,138.9060,137.9067,139.9053,141.9093,137.9060,135.9071,								TABL2250		
C		PR 190	ND 191	192	193	194	195	196	TABL2260		
M	140.9075,141.9075,143.9098,145.9127,142.9096,144.9121,147.9165,								TABL2270		
C		197	SM 198	199	200	201	202	203	TABL2280		
M	149.9208,151.9194,153.9219,146.9145,148.9168,147.9144,149.9169,								TABL2290		
C		204	EV 205	206	CE 207	208	209	210	TABL2300		
M	143.9117,152.9206,150.9195,157.9244,159.9272,155.9223,156.9241,								TABL2310		
C		211	212	213	TB 214	DY 215	216	217	TABL2320		
M	154.9227,153.9209,151.9194,158.9249,163.9285,161.9256,162.9278,								TABL2330		
C		218	219	220	221	HO 222	ER 223	224	TABL2340		
M	160.9257,159.9239,157.9240,155.9140,164.9291,165.9287,167.9308,								TABL2350		
C		225	226	227	228	TM 229	YR 230	231	TABL2360		
M	166.9305,169.9356,163.9298,161.9287,168.9343,173.9256,171.9252,								TABL2370		
C		232	233	234	235	236	LU 237	238	TABL2380		
M	172.9380,170.9360,175.9427,169.9340,167.9339,174.9420,175.9419,								TABL2390		
C		HF 239	240	241	242	243	244	TA 245	TABL2400		
M	179.9461,177.9430,176.9425,178.9452,175.9408,173.9390,180.9458,								TABL2410		
C		246	W 247	248	249	250	251	RE 252	TABL2420		
M	179.9450,183.9489,185.9507,181.9460,182.9481,179.9445,186.9530,								TABL2430		
C		253	OS 254	255	256	257	258	259	TABL2440		
M	184.9480,191.9622,189.9548,188.9585,187.9569,186.956,185.952,								TABL2450		
C		260	IR 261	262	PT 263	264	265	266	TABL2460		
M	183.946,192.9667,190.9634,194.9662,193.9633,195.9671,197.9646/								TABL2470		
	DATA TMC2/								TABL2480		
C		267	268	AU 269	HG 270	271	272	273	TABL2490		
M	191.9648,189.964,196.9672,201.9706,199.9683,198.9682,200.9703,								TABL2500		
C		274	275	276	TL 277	278	PR 279	280	TABL2510		
M	197.9667,203.9735,195.9658,204.9738,202.9719,207.9766,205.9744,								TABL2520		
C		281	282	BI 283	RA 284	TH 285	PA 286	U 287	TABL2530		
M	206.9759,203.9731,208.9793,226.0254,232.0382,231.0359,238.0486,								TABL2540		
C		288	289	NP 290	PU 291				TABL2550		
M	235.0428,234.0403,237.0480,239.0522/								TABL2560		
	DATA MS/								TABL2570		
C		1	2	3	5	7	8	10	12	14	TABL2580
N	'H', 'H2',2*'HE',2*'LI', 'BE',2*'B',2*'C',2*'N',3*'O',										TABL2590
C		17	18	21	22	25	26	29	30	34	TABL2600
N	'F',3*'NE', 'NA',3*'MG', 'AL',3*'SI', 'P',4*'S',2*'CL',										TABL2610
C		36	39	42	48	49	54	56	60	61	TABL2620
N	3*'AR',3*'K',6*'CA', 'SC',5*'TI',2*'V',4*'CR', 'MN',4*'FE',										TABL2630
C		65	66	71	73	78	80	85	86	92	TABL2640
N	'CO',5*'NI',2*'CU',5*'ZN',2*'GA',5*'GE', 'AS',6*'SE',2*'BR',										TABL2650
C		94	100	102	106	107	112	113	120	127	TABL2660
N	6*'KR',2*'RB',4*'SR', 'Y',5*'Zr', 'NB',7*'MO',7*'RU', 'R',										TABL2670
C		128	134	136	144	146	156	158	166	167	TABL2680
N	6*'PD',2*'AG',8*'CD',2*'IN',10*'SN',2*'SB',8*'TE', 'I',9*'XE',										TABL2690
C		176	177	184	186	190	191	198	205	207	TABL2700
N	'CS',7*'BA',2*'LA',4*'CE', 'FR',7*'ND',7*'SM',2*'EU',7*'GO',										TABL2710
C		214	215	222	223	229	230	237	239	245	TABL2720

```

N      'TB',7*'DY', 'HO',6*'ER', 'TM',7*'YB',2*'LU',6*'HF',2*'TA', TABL2730
C      247 252 254 261 263 265 270 277 279 TABL2740
N      5*'W',2*'RE',7*'CS',2*'IR',6*'PT', 'AU',7*'HG',2*'TL',4*'PB', TABL2750
C      283 284 285 286 287 290 291 TABL2760
N      'BI', 'RA', 'TH', 'PA',3*'L', 'NP', 'PU' TABL2770
      END TABL2780

```

```

SUBROUTINE INTERP(X,Y,IUP,NP,XIN,YOUT)
DIMENSION X(1),Y(1)
6      DO 10 I=1,IUP
      IF (XIN-X(I))11,60,10
10     CONTINUE
11     IN=I-NP/2-1
      IF (IN)15,20,20
15     IN=0
      GO TO 30
20     IF (IN+NP-IUP)30,30,25
25     IN=IUP-NP
30     YCUT=0.
      DO 40 I=1,NP
      ANUM=1.
      DEN=1.
      INI=IN+I
      DC 38 J=1,NP
      IF (I-J)32,38,32
32     INJ=IN+J
      ANUM=(XIN-X(INJ))*ANUM
      DEN=(X(INI)-X(INJ))*DEN
38     CONTINUE
40     YOUT=ANUM*Y(INI)/DEN+YCUT
50     RETURN
60     YOUT=Y(I)
      RETURN
      END

```

```

SUBROUTINE ZERL(I1,N)
DIMENSION I1(1)
5      DO 5 I=1,N
      I1(I)=C
      RETURN
      END

```

Definition of Variables.

1. Main Program (MASP)

A	- TAIN (K1) - abundance of a given nuclide (see B)
AIB	- array of relative background intensities as read from calibration curve
AIN	- corresponding abundance for each entry in the IN array
AIP	- array of relative peak intensities as read from calibration curve
AIS	- isotopic abundance of internal standard
AMAX	- sorted maximum
AMIN	- sorted minimum
ANC	- array of relative peak intensities
ATWT	- array of atomic weights corresponding to the ISYM and SENS arrays
AVDEV	- average deviation
AVG	- average (SUM/FI)
B	- TAIN (K2) - abundance of a given nuclide (see A)
BLANK	- 1077952576
C	- array of line concentrations
CIN	- array of concentrations of solved ions or clusters (includes named masses)
CLA	- array of abundance for each isotope (clusters)
CLM	- array of mass for each isotope (clusters)
CLMOZ	- mass of multiply charged cluster
CL1	- array of first name of each isotope for clusters
CL2	- array of second name of each isotope for clusters

COMNT	- optional comment on impurity card
CON	- concentration of a particular line
DLAB	- 20 character data label on plot
E	- array of possible exposure values used for calculating concentrations
EOVN	- ratio of exposure value to line intensity - E/ANC (an array)
EVONS	- average ratio of exposure value (E) to line intensity (N) = SUM/FI where SUM is sum of all EOVN and FI is number of EOVN
FI	= NEXP - number of exposures
FIN	= IN(I, J)
GLAB	- 20 character graph label on plot
IC	- array of charge of each names mass
ICG	- charge of named ion or cluster
ICL	- switch for charge on names and unnamed clusters
IE	- exposure index of E
IEL1	- first part of name of particular cluster or ion in sensitivity section of program
IEL2	- second part of name of a particular cluster or ion in sensitivity section of program
IEND	- the word 'END' on a card at the end of each data set
IES	- default exposure index (exposure number of default control
IGO	- switch
IIE	- an array of exposure indices of a nominal mass
IN	- two dimensional array of pointers to possible ions for each unknown spectra line
ION	- array of composite names of cluster components to be added to tables

ISYM	- array of symbols for each element or cluster
IUP	= NP1 - number of elements in an array to be interpolated
IZ	- pen up or down parameter of subroutine PLOT
JC	- a particular value of charge
JC2	- maximum charge for clusters
LAST	- value $\neq 0$ indicates last line determination for this mass
LC	- maximum charge on ion for which the program will search
LCL1	- array of first half of input name for each listed cluster
LCL2	- array of second half of input name for each listed cluster
LCS	- maximum charge searched on matrix (main constituent ion)
LGO	- indicator for type (1 or 2)
LH	- indicator of relative mass position for multiple lines (low, high, intermediate)
LIN	- array to which elements of IN point, also a pointer in the decimal form: $\pm JJIII$ where: the sign is negative for a cluster and is positive for a non-cluster ion, JJ is the charge of the ion or cluster, and III is an index of MS and associated arrays for ions as well as an index of CL1 and CL2 and associated arrays for clusters
MS	- array of symbols for naturally occurring nuclides
N	- variable exponent of RO
NAME	- name of matrix element
NAME1	- first part of name of cluster or ion used to solve equations
NAME2	- second part of name of cluster or ion used to solve equations
NAM1	- first half of name of ion or cluster on mass card
NAM2	- second half of name of ion or cluster on mass card
NCL	- number of clusters

NCLC	- number of cluster component cards
NCL1	- name of first cluster component
NCL2	- name of second cluster component
NE	- number of exposure values
NEQ	- number of equations
NEXP	- number of exposures used at a given mass
NI	- number of ions at a mass before eliminations begin
NIN	- number of ions
NIT	- number of items in ion tables (291 nuclides and cluster component additions)
NI1	- number of ions at a mass after eliminations are completed
NM	- number of mass vs position pairs
NMC	- number of mass cards
NN	- an array representing uncombined cluster ions in sequence
NNAM, NNM	- number of named masses
NP	- number of peaks with the same mass
NSENS	- number of relative sensitivity changes
NTE	- number of data points for preliminary curve
NTEQ	- total number of equations
NT1	- array for first half of names of named masses
NT2	- array for second half of names of named masses
NUN	- index in the cluster tables where the named clusters end and the unnamed clusters begin
N1	- number of times first half of cluster component is used (cols. 4 & 5)
N2	- number of times second half of cluster component is used (cols. 9 & 10)

PCDEV - percent average deviation for EOVN values
 PCTDV - percent average deviation for concentration values
 PLT - value $\neq 0$ calls for plot of calibration curve
 PLTDN = TDN/10; array for plotting vs R
 POS - position data on mass vs position cards (an array)
 PPMA - ppm atomic concentration for a particular ion or cluster
 PPMW - ppm by weight concentration for a particular ion or cluster
 PSN - position data on mass card
 R = RO**(II-1); II=2, NP1 (an array)
 REMKS - 20 characters used for sample identification
 RLOG - R array to be plotted vs TDN
 RO - ratio of calibrating isotopes
 SENS - array used for relative sensitivity values
 SGN - negative if either cluster component contains hydrogen
 SMASS - mass of internal standard
 SPMA - ppm atomic corrected by sensitivity factor
 SPMW - ppm by weight corrected by sensitivity factor
 SPUNC - numerator of default uncertainty for position data
 SPUNC1 - denominator of (or) default uncertainty for position data
 SQRTMS - mass data on mass vs position cards (an array)
 SS - relative sensitivity of internal standard
 STMAS - atomic mass used to convert ppm atomic to ppm by weight
 SUNC - numerator of default uncertainty for mass data
 SUNC1 - denominator of (or) default uncertainty for mass data

TA	- temporary abundance tables (an array)
TAIN	- array of abundances for each nuclide
TB	- array of transmissions of background adjacent to spectral line
TBS	- default background transmission
TD	- array of optical transmissions of more abundant isotope (dark line)
TDN	- array of points (TD2) read from transmission curve used to plot calibration curve
TD1	- starting transmission point of calibration curve generation
TD2	- point on transmission curve corresponding to TD1
TL	- array of optical transmissions of less abundant isotope (light line)
TM	- temporary mass tables (an array)
TMC	- array of mass values for each nuclide
TP	- array of minimum transmissions of spectral line (peak)
TWT	- computed atomic weight
UC	- concentration at a particular mass
UCI	- array of line intensities (concentrations)
UL1	- default upper limit
UM	- array of masses for each named ion
UMASS	- mass of spectral line (also negative mass area)
UMN	- array of unknown masses
UN	- array of uncertainties for each mass
UNC	- cols. 13-20 on mass card (used for negative mass and uncertainty)

UNCL - col. 11 on mass card (numerator for uncertainty)
 UN1 - array of uncertainties for each named mass
 W - line width array
 WIN - array of atomic weights corresponding to each LIN element
 XLAB - 20 character label along X-axis of plot
 YLAB - 20 character label along Y-axis of plot

2. ZERO. This is a routine used to zero a section of core. The first parameter is the array to be zeroed and the second is the number of elements.

3. INTERP. An interpolation routine using the Lagrangian formula. The X array must be ordered.

4. Subroutine CONC. Determines the concentration for any mass called for. It is always taken as the darker of any multiplet lines.

W - input mass to be interrogated

UC - concentration at mass W.

If there is no nominal mass at $W \pm$ an uncertainty, then UC is returned as zero.

5. Subroutine PRINT. Used solely for printing the equations in the desired format.

6. Subroutine MUCH. This is a combination multicharge-isotopic abundance test. L1, L2, L3 - (see LIN in main program).

C - concentration of the weakest line at the tested nominal mass

Y - testing charge which carries from 1 to Z

- Z - charge of possible ion being tested
- REJ - percentage concentration level below which the ion is
 rejected (.1)
- AIR - ratio of abundances of isotopes of ion being tested
- UC - concentration of strongest line within mass uncertainty.

Each ion is put to the following test for each of its isotopes at the same charge and for each lesser charge. If $.5^{**}(Z-Y)*AIR*UC < REJ*C$ then delete the ion being tested as possibility at that mass. If $UC=0$ then it is set equal to the upper limit (UL1) for type 1 data ($LGO=1$), or the test is ignored for type 2 data ($LGO=2$), where the information taken was incomplete.

7. Subroutine HYCA. Performs a specific test on all clusters containing hydrogen.

- IB, IC, ID - (see LIN in main program)
- WT - weight of the +1 charged ion less one hydrogen mass
- C - concentration of the weakest line at the mass being
 tested
- W - weight at each charge tested up to IB

8. Subroutine SIMUL. For this program, an assumption was made that each question would never contain more than 15 unknowns. Thus the array was set at 300×15 so that two arrays with a total of 9000 entries replaced the more general but far less tractable array with 90,000 entries. Two of these arrays are needed since there must be one for the coefficients and one for the unknowns associated with the coefficients. The unknown array contains an index (or pointer) to other descriptive arrays.

Another assumption was made on the basis of the limited deviation of isotopic masses from the atomic weight. Thus, with the proper ordering of rows and columns, a quasi-Gaussian elimination procedure could be used without encountering more than 15 unknowns in one equation throughout the elimination process. In this subroutine the ordering is done by atomic weight with the exception of named masses (knowns) which are placed first in the matrix.

The Gaussian elimination procedure contains some items which are designed to give optimum use of information. As each unknown is encountered in the forward solution, the next several equations are scanned for this unknown to determine the isotope on which to pivot (i. e. for use in elimination from other equations). The isotope with the largest abundance (assumed to contain more accurate intensity information) is chosen unless an equation is found which contains only one unknown. This isotope is then used to pivot on if its abundance (coefficient) is at least 20 percent of the isotope with the largest abundance.

In the backward solution, the last unknown in each equation is used as the pivot. The procedure allows some unknowns to be overspecified (in which case the unsolvable unknowns are returned). The solution to the equations are listed under the heading "Solved Equations" in the form of a number representing the atomic concentration in ppm for the ion or ions that follow.

- A - banded matrix
- M - subscript matrix for A
- NE - number of equations
- V - vector for solution

9. Subroutine TABLE. This is a block data compilation used for initialing six arrays and is non-executable.
10. Function ILF. A machine language routine which converts an integer into an A4 format.
11. LABEL. This routine must be the first plotting subroutine called for the ISU plotting system. It initializes and labels plots and is non Cal Comp.
12. PLOT. Basic subroutine which moves the pen to the point (X, Y)
13. SYMBOL. Generates annotation and also includes special symbols to use for plotting points.
14. AXIS. Draws an axis with associated annotations and labels.
15. LINE. Connects the points in arrays with straight lines.
16. ENDPLT. This routine (actually an added entry of PLOT) must be the last plotting subroutine called and writes some accounting information for the local system. It is non Cal Comp.

EXAMPLE

To illustrate how the program is used, it is applied to the data from a sample of thorium metal. The mass spectrum was obtained and features on the photoplate were measured on a microdensitometer. The variety of forms which the input can take are given first followed by the output from the computer which a trained operator uses to obtain sample impurity levels.

Input

Input data consists of 15 different possible sets of cards. Only those sets followed by an asterisk are required, the others being optional. The variables within a set which are required in order to run the program are also denoted by an asterisk. Actual card examples are shown at the end of each set.

MAASP Formats

		<u>Number</u>	<u>Columns</u>
I.	Calibration Curve Control (1 card)*		
A.	NTE*	integer	1-10
B.	N*	"	11-20
C.	RO*	real	21-30
D.	TD1*	"	31-40
E.	PLT - if $\neq 0$, plot will be made	"	41-50

II. Calibration Curve Data (4 sets per card)*

A.	TL - transmission of light line*	real	1-10, 21-30 41-50, 61-70
B.	TD - transmission of dark line*	"	11-20, 31-40 51-60, 71-80

III. Calibration Curve Plot (1 card)

A.	XLAB - X-axis label	alphanumeric	1-20
B.	YLAB - Y-axis label	"	21-40
C.	GLAB - Graph label	"	41-60
D.	DLAB - Data label	"	61-80

IV. Standard Reference Control (1 card)*

A.	NE - number of exposures*	integer	1-10
B.	SMASS - mass of reference isotope*	real	11-20
C.	ALS - abundance of reference isotope*	"	21-30
D.	SS - relative sensitivity of reference	"	31-40
E.	NAME - symbol of matrix element*	alpha	41-44

F.	LCS - maximum number of charges on matrix element*	integer	45-46
G.	STMAS	real	51-60
H.	REMK5	alphameric	61-80

[illegible]

V. Exposure Value Data (8 per card)*

A. E - exposure value in coulombs exponential 1-10, 11-21,
21-30, ...

[illegible]

VI. Reference Data (1 set per card)*

A.	TP - peak transmission*	real	41-50
B.	TB - background transmission*	"	51-60
C.	W - line width*	"	61-70
D.	IE - exposure number*	integer	71-72
E.	LAST - if last line read, put 1 here	"	80

[illegible]

VII. Default Control (1 card)*

A.	LGO = 1 if all data taken = 2 if only part of data was taken	integer	1
B.	NM - number of mass <u>vs</u> position sets	"	2-5
C.	SUNC, SUNC1 - default mass uncertainty if written as decimal, use cols 13-20*	real	11-20
D.	SPUNC, SPUNC1 - default position uncertainty if written as decimal, use cols 23-30	real	21-30
E.	LC - maximum number of charges on an ion*	integer	31-35
F.	TP - upper limit peak transmission*	real	41-50
G.	TB - default (upper limit) background transmission*	real	51-60
H.	W - upper limit line width (same as reference line)*	real	61-70
I.	IE - number of longest exposure*	integer	71-72

VIII. Mass vs Position Data (4 sets per card)

A.	SQR TMS - exact mass	real	1-10, 21-30 41-50, 61-70
B.	POS - exact position of preceding mass	"	11-20, 31-40, 51-60, 71-100

IX. Transmission data (A thru E required on 1st card of each set of lines of same mass)*

A.	UMASS - mass in ascending order	real	1-10
B.	UNCL, UNC - uncertainty, mass or position, fraction or decimal, if decimal start in col. 13	real	11-20
C.	PSN - position if mass is unknown	real	21-30
D.	NAM1, NAM2 - name of ion or cluster in proper format	alpha	31-38
E.	ICG - charge of ion cluster	integer	39-40
F.	TP - peak transmission*	real	41-50
G.	TB - background transmission	"	51-60
H.	W - line width	"	61-70
I.	IE - exposure number	"	71-80
J.	COMNT - comments (1 card only, any card)	alphameric	73-79
K.	LAST - = 1 indicates last line at this mass	integer	80

[illegible]

X. Blank card (indicates end of transmission data)*

XI. Cluster and sensitivity control (1 card)

A.	NCLC - number of cluster ion cards	integer	1-10
B.	NCl - number of clusters	"	11-20
C.	NSENS - number of sensitivity changes	"	21-30

[illegible]

XII. Cluster Ions (up to 14 per card)

A.	NCL1 - name of first ion	alphameric 1-3
B.	N1 - number of first ion	integer 4-5
C.	NCL2 - name of second ion	alphameric 6-8
D.	N2 - number of second ion	integer 9-10

E.	ION - names of ion formed by successive combinations of names given	alphameric 11-14, 16-19 21-24, 26-29 ...
----	---	--

[illegible]

XIII. Clusters (8 per card)

A.	LCL1 - name of first part of cluster	alpha	1-4, 11-14 21-24, ...
B.	LCL2 - name of second part of cluster	"	5-8, 15-18, 25-28, ...

[illegible]

XIV. Sensitivity changes (8 per card)

A.	NT1 - name of ion whose sensitivity alpha is to be changed		1-4, 11-14, 21-24, ...
B.	UN1 - new sensitivity	real	5-10, 15-20, 25-30, ...

[illegible]

XV. End of data set*

- A. Write END (left justify)* alpha 1-4
- B. Blank card at end followed
by /*card*

OUTPUT

Usually the final listing of ions and concentration is not in appropriate form for direct transmission to the customer. A trained individual can quickly review the various readouts and make a complete report of the impurity elements. The following readouts are obtained: 1. Listing of pertinent plate information including calibration curve data, reference line data, mass, and intensity data, 2. Gross Equations, 3. Net Equations, 4. Solved Equations, and 5. Final listing of ion and concentration.

Output Example

CALIBRATION CURVE - 19 18 2.CCCCC 5.6337? MASP VERSION 1 AUG 1967

STANDARD - 4 232.00000 1.00000000 1.00000 TH +14 232.03999 178-517A TH METAL

AVERAGE ES/NSC = C.71011751E-15 AVERAGE DEVIATION = 0.88785464E-16 PCT DEV = 12.50

0.62296436E-15 C.64896554E-15 0.88785464E-15 C.68025271E-15

DEFAULT UPPER LIMIT IS C.COC104

MASS	CMNT	PCT DEV	AVG C(I)	C(I)S VS EXP				
8.000		16.103	11.740	5.849 10	13.620	9		
9.000		0.0	0.040	0.040 12				
9.330		0.000	2.492	-11.757 1	2.492	11		
9.650		0.0	0.081	C.081 12				
10.000	LCW MASS	0.0	0.051	0.051 12				
10.000	HEW MASS	0.0	0.048	C.048 12				
10.330		0.0	0.045	0.045 12				
10.670		0.0	0.034	0.034 12				
11.000		0.0	0.331	0.331 12				
12.000		15.315	323.912	323.890 9	233.514	7	315.096	2 419.147 E
13.000		0.0	9.736	9.736 10				
13.500		0.0	C.120	0.120 12				
14.000		8.324	97.612	101.719 2	106.782	9	81.362	7 100.586 E
14.500		0.0	0.949	0.949 11				
15.000		0.0	0.704	0.704 11				
15.000		0.0	0.583	0.583 11				
15.000		0.0	46.242	46.242 10				
15.500		0.0	0.489	C.489 11				
16.000		0.0	267.789	267.789 8				
16.000		0.0	35.201	35.201 9				
16.570		0.0	C.097	C.097 12				
17.000		0.0	0.205	0.205 12				
17.000		0.0	C.389	C.389 12				
17.000		0.0	0.216	0.216 12				
17.330		0.0	0.081	C.081 12				
17.500		0.0	0.127	0.127 12				
17.849		0.0	0.860	C.860 12				
18.000		0.0	3.107	3.107 12				
18.500		0.0	0.045	0.045 12				
18.670		0.0	C.084	0.084 12				
19.000		0.0	0.043	0.043 12				
19.300		0.0	0.141	0.141 12				
19.336		0.0	3.055	3.055 11				
20.000		0.0	0.348	0.348 12				
21.094		0.0	9.303	9.303 10				
22.500		0.0	1.179	1.179 12				
23.000		0.0	1.258	1.258 12				
23.200		0.0	36.090	36.090 10				
24.000		0.0	C.225	0.225 12				
24.000		0.0	0.308	0.308 12				
25.000		0.0	C.443	C.443 12				
25.500		0.0	2.199	2.199 12				
25.780		0.0	67.830	67.830 9				
26.000		0.0	C.475	0.475 12				
26.000		0.0	2.264	2.264 12				
26.500		0.0	C.034	0.034 12				
27.000		0.0	5.632	5.632 12				
27.000		0.0	1.369	1.369 12				

28.000		0.0	317.554	317.554	9		
28.000	HIGH	14.073	2.214	1.760	10	2.202	11
29.000		0.0	9.086	9.086	9		2.662 12
29.000		0.0	328.030	328.030	9		
30.000		0.0	5.538	5.538	11		
31.000		0.0	8.428	8.428	11		
32.000		0.0	5.985	5.985	11		
33.000		0.0	0.066	0.066	12		
33.148		0.0	405.245	405.245	8		
34.000		0.0	0.314	0.314	12		
35.000		0.0	2.287	2.287	12		
36.000		0.0	0.133	0.133	12		
36.200		0.0	0.881	0.881	12		
37.000		0.0	0.544	0.544	12		
37.000		0.0	0.128	0.128	12		
38.000		0.0	0.126	0.126	12		
38.670		0.0	1334.875	1334.875	7		
39.000		0.0	0.245	0.245	12		
39.000		0.0	0.354	0.354	12		
40.000		0.0	2.075	2.075	12		
40.000		0.0	0.070	0.070	12		
41.000		0.0	0.123	0.123	12		
42.000		0.0	0.083	0.083	12		
43.000		0.0	0.028	0.028	12		
43.976		0.0	0.598	0.598	12		
44.453		0.0	0.124	0.124	12		
44.947		0.0	11.796	11.796	11		
45.237		0.0	5.964	5.964	12		
45.454		0.0	0.162	0.162	12		
45.938		0.0	0.564	0.564	12		
46.400		0.0	8964.238	8964.238	7		
46.935		0.0	0.414	0.414	12		
47.938		0.0	1.253	1.253	12		
48.951		0.0	0.131	0.131	12		
49.002		0.0	0.038	0.038	12		
49.939		0.0	0.192	0.192	12		
49.956		0.0	0.108	0.108	12		
50.942		0.0	6.135	6.135	11		
51.923		0.0	2.394	2.394	12		
52.929		0.0	0.193	0.193	12		
53.945		0.0	0.229	0.229	12		
54.933		0.0	0.155	0.155	12		
55.935		0.0	4.848	4.848	12		
56.918		0.0	0.123	0.123	12		
58.000		0.0	22106.312	22106.312	6		
59.918		0.0	2.685	2.685	12		
60.309		0.0	1.659	1.659	12		
60.639		0.0	0.167	0.167	12		
60.924		0.0	0.200	0.200	12		
61.318		0.0	0.229	0.229	12		
61.915		0.0	0.300	0.300	12		
61.978		0.0	0.232	0.232	12		
62.319		0.0	0.145	0.145	12		
64.000		0.0	0.113	0.113	12		
65.000		0.0	0.054	0.054	12		
75.000		0.0	0.384	0.384	12		
77.330		0.0	219708.437	219708.437	6		
89.000		0.0	0.536	0.536	12		
90.000		0.0	4.244	4.244	12		
90.500		0.0	71.250	71.250	11		
91.000		0.0	0.742	0.742	12		
91.000		0.0	1.392	1.392	12		
91.500		0.0	0.727	0.727	12		
92.000		0.0	1.293	1.293	12		
92.000		0.0	2.094	2.094	12		
92.500		0.0	0.568	0.568	12		

93.000	0.0	8.211	8.211	11
93.500	0.0	0.893	0.893	12
94.000	0.0	1.630	1.630	12
96.000	0.0	0.262	0.262	12
115.000	0.0	0.811	0.811	12
116.000	0.0	752868.812	752868.812	4
116.500	0.0	16.811	16.811	12
122.000	0.0	1.365	1.365	12
122.500	0.0	0.299	0.299	12
123.000	0.0	0.474	0.474	12
124.000	0.0	12.513	12.513	12
NEGATIVE FROM MASS-170.00 TO MASS-180.00 UP.LIM.				0.44
181.000	0.0	176.418	176.418	11
182.000	0.0	4.631	4.631	12
183.000	0.0	2.465	2.465	12
184.000	0.0	4.927	4.927	12
185.000	0.0	2.358	2.358	12
186.000	0.0	4.847	4.847	12
187.000	0.0	4.484	4.484	12
232.000	0.0	1066693.000	1066693.000	4
233.000	0.0	561.180	561.180	10
234.000	0.0	9.969	9.969	12
235.000	0.0	7.285	7.285	12
NEGATIVE FROM MASS-236.00 TO MASS-237.00 UP.LIM.				1.26
238.000	0.0	1.405	1.405	12
NEGATIVE FROM MASS-238.20 TO MASS-240.00 UP.LIM.				1.08
244.000	0.0	90.948	90.948	11
245.000	0.0	5.990	5.990	12
246.000	0.0	8.613	8.613	12
248.000	0.0	949.914	949.914	10
249.000	0.0	17.252	17.252	12
250.000	0.0	3.104	3.104	12
256.000	0.0	5.534	5.534	12
257.000	0.0	1.206	1.206	12
264.000	0.0	10.974	10.974	12

178-517# TH METAL TYPE 1

62

22.500	1.1787 = 0.5146	ZP	+ 4	+ 1.0000	SC	+ 2	+ C.0118C	C2	+ 2	+					
23.000	1.2578 = 0.1711	ZP	+ 4	+ C.0800	TI	+ 2	+ 0.0000	CA	+ 2	+ C.1584	MO	+ 4	+ 1.0000	NA	+ 1
	+ 0.0040C														
23.200	36.0502 = 1.0000	TH	+ 1C	+											
24.000	0.2247 = 0.7398	TI	+ 2	+ 0.1653	MO	+ 4	+ 0.0018	CA	+ 2	+ 0.0551	RU	+ 4	+ 0.0280	ZR	+ 4
	+ 0.7870	MG	+ 1	+ 0.9780	C2	+ 1	+ 0.9564	C4	+ 2	+					
24.000	0.3081 = 0.0		+ 0	+											
25.000	0.4427 = 0.0534	TI	+ 2	+ 0.0431	CR	+ 2	+ 0.0024	V	+ 2	+ 1.0000	AS	+ 3	+ 0.1013	MG	+ 1
	+ 0.0219	C2	+ 1	+ 0.0007	C4	+ 2	+ -0.0428C4	H	+ 2	+ -0.9780	C2H	+ 1	+ -0.9564C4	F2	+ 2
25.500	2.1594 = 0.9976	V	+ 2	+ -0.0007C4	F	+ 2	+ -0.0428C4	H2	+ 2	+					
26.000	0.4751 = 0.8376	CR	+ 2	+ C.1117	MG	+ 1	+ 0.0001	C2	+ 1	+ -0.0219	C2H	+ 1	+ -C.0007C4	F2	+ 2
	+ -0.9780	C2H2	+ 1	+											
26.000	2.2644 = 0.0		+ 0	+											
26.500	0.0343 = 0.0555	CR	+ 2	+											
27.000	5.6320 = 1.0000	AL	+ 1	+ -C.0001	C2H	+ 1	+ -0.0219	C2H2	+ 1	+ -0.5780	C2H3	+ 1	+		
27.000	1.3650 = 0.0		+ 0	+											
28.000	317.5537 = 0.9221	SI	+ 1	+ 0.9865C	C	+ 1	+ -0.0001	C2H2	+ 1	+ -0.0219	C2H3	+ 1	+ -C.5780	C2H4	+ 1
	+														
28.000	2.2143 = 0.0		+ C	+											
29.000	9.0856 = 0.0033	FE	+ 2	+ 0.6788	NI	+ 2	+ 0.1430	SN	+ 4	+ 0.0758	CO	+ 4	+ C.0470	SI	+ 1
	+ 0.0114C	D	+ 1	+ 1.0000	TH	+ 8	+ -0.0001	C2H3	+ 1	+ -0.0219	C2H4	+ 1	+ -0.9780	C2H5	+ 1
29.000	328.0298 = 0.0		+ C	+											
30.000	9.5376 = 0.2623	NI	+ 2	+ 0.5146	ZR	+ 3	+ 0.0309	SI	+ 1	+ C.0020C	D	+ 1	+ -0.0001	C2H4	+ 1
	+ -0.0219	C2H5	+ 1	+ -0.9780	C2H6	+ 1	+								
31.000	8.4282 = 1.0000	NB	+ 3	+ 1.0000	P	+ 1	+ 0.0461	TE	+ 4	+ 0.0594	SN	+ 4	+ 0.0001	XE	+ 4
	+ 0.0000C	D	+ 1	+ -0.0001	C2H5	+ 1	+ -0.0219	C2H6	+ 1	+					
32.000	5.9854 = 0.9500	S	+ 1	+ 0.9952	C2	+ 1	+ -0.0001	C2H6	+ 1	+					
33.000	0.0663 = 0.0076	S	+ 1	+ 0.0007	C2	+ 1	+								
33.148	405.2451 = 1.0000	TH	+ 7	+											
34.000	0.3138 = 0.0422	S	+ 1	+ 0.0041	O2	+ 1	+								
35.000	2.2868 = 0.7553	CL	+ 1	+											
36.000	0.1330 = 0.0001	S	+ 1	+ 0.0024	AR	+ 1	+ 0.9672	C3	+ 1	+					
37.000	0.5442 = 0.2447	CL	+ 1	+ C.0325	C3	+ 1	+ -0.9672C3	H	+ 1	+					
37.000	0.1276 = 0.0		+ C	+											
38.000	0.1263 = 0.0006	AR	+ 1	+ C.0004	C3	+ 1	+ -0.0325C3	H	+ 1	+ -0.9672C3	H2	+ 1	+		
38.670	1334.8752 = 0.1430	SN	+ 3	+ 0.0758	CO	+ 3	+ 1.0000	TH	+ 6	+					
39.000	0.2446 = 0.9310	K	+ 1	+ -0.0004C3	H	+ 1	+ -0.0325C3	H2	+ 1	+ -0.9672C3	H3	+ 1	+		
39.000	0.3545 = 0.0		+ 0	+											
40.000	2.0750 = 0.9960	AR	+ 1	+ C.9697	CA	+ 1	+ 0.0001	K	+ 1	+ 0.9756C2	D	+ 1	+ -0.0004C3	F2	+ 1
	+ -0.0325C3	H3	+ 1	+ -0.9572C3	F4	+ 1	+								
40.000	0.0703 = 0.0		+ 0	+											
41.000	0.1232 = 0.0688	K	+ 1	+ 0.4275	SE	+ 3	+ 0.0007	TE	+ 3	+ 0.0222C2	D	+ 1	+ -0.0004C3	F3	+ 1
	+ -0.0325C3	H4	+ 1	+ -0.9672C3	H5	+ 1	+								
42.000	0.0828 = 0.0064	CA	+ 1	+ C.0021C2	C	+ 1	+ -0.0004C3	H4	+ 1	+ -0.0325C3	H5	+ 1	+ -0.9672C3	F6	+ 1
	+														
43.000	0.0284 = 0.0015	CA	+ 1	+ 0.2182	YB	+ 4	+ 0.0000C2	D	+ 1	+ -0.0004C3	H5	+ 1	+ -0.0325C3	F6	+ 1
	+														
43.976	0.5983 = 0.0206	CA	+ 1	+ 0.9842C	O2	+ 1	+								
44.453	0.1244 = 1.0000	Y	+ 2	+											
44.947	11.7958 = 0.5146	ZR	+ 2	+ 1.0000	SC	+ 1	+								
45.237	5.9635 = 0.9999	TA	+ 4	+											
45.454	0.1621 = 0.1122	ZR	+ 2	+											
45.938	0.5644 = 0.1711	ZR	+ 2	+ 0.0800	TI	+ 1	+ 0.0000	CA	+ 1	+ 0.1584	MO	+ 2	+		
46.400	8564.2383 = 1.0000	TH	+ 5	+											
46.935	0.4137 = 0.0729	TI	+ 1	+ 0.0904	MO	+ 2	+ 0.1740	ZR	+ 2	+					
47.938	1.2530 = 0.7398	TI	+ 1	+ 0.1653	MC	+ 2	+ 0.0018	CA	+ 1	+ 0.0551	RU	+ 2	+ 0.0280	ZR	+ 2
	+														
48.951	0.1307 = 0.0551	TI	+ 1	+											
49.002	0.0379 = 0.0428	C4	+ 1	+ -0.9564C4	F	+ 1	+								
49.939	0.1521 = 0.0534	TI	+ 1	+ 0.0431	CR	+ 1	+ 0.0024	V	+ 1	+					
49.996	0.1075 = 0.0007	C4	+ 1	+ -0.0428C4	F	+ 1	+ -0.9564C4	H2	+ 1	+					
50.942	6.1347 = 0.9976	V	+ 1	+											
51.923	2.3936 = 0.8376	CR	+ 1	+											
52.929	0.1930 = 0.0555	CR	+ 1	+											
53.945	0.2295 = 0.0238	CR	+ 1	+ 0.0582	FE	+ 1	+								
54.933	0.1554 = 1.0000	MA	+ 1	+											

55.935	4.8484 = 0.5166	FE + 1 +						
56.518	0.1227 = 0.0219	FE + 1 -						
58.000	22106.3125 = 0.0033	FE + 1 + 0.6783	NI + 1 + 0.1430	SA - 2 + 0.0758	CC + 2 + 1.0000	TH + 4		
59.918	2.6647 = 0.2623	NI + 1 -						
60.309	1.6587 = 0.9999	TA + 3 +						
60.635	0.1673 = 0.2641	h + 3 +						
60.924	0.2002 = 0.0119	NI + 1 + 0.0246	TE + 2 + 0.0472	SN + 2 +				
61.318	0.2287 = 0.0002	CS + 3 + 0.3064	h + 3 +					
61.915	0.3001 = 0.0366	NI + 1 +						
61.978	0.2324 = 0.0461	TE + 2 + 0.0554	SN + 2 + 0.0001	XE + 2 + 0.2841	W + 2 + 0.0159	CS + 3		
62.319	0.1488 = 0.6293	RE + 3 + 0.0164	OS + 3 +					
64.000	0.1131 = 0.0108	NI + 1 + 0.4885	ZN + 1 +					
65.000	0.0542 = 0.3091	CU + 1 +						
75.000	0.3835 = 1.0000	AS + 1 +						
89.000	0.5361 = 1.0000	Y + 1 + 0.2714	PF + 2 +					
90.000	4.2437 = 0.5146	ZR + 1 +						
90.500	71.2502 = 0.5599	TA + 2 +						
91.000	0.7420 = 0.1122	ZR + 1 + 0.2641	W + 2 +					
91.000	1.3516 = 0.0	+ 0 +						
91.500	0.7269 = 0.1440	h + 2 +						
92.000	1.2527 = 0.1711	ZR + 1 + 0.1584	MO + 1 + 0.0002	OS + 2 + 0.3064	W + 2 +			
92.000	2.0944 = 0.0	h + 0 +						
92.500	0.5680 = 0.3707	RE + 2 +						
93.000	8.2110 = 1.0000	WB + 1 + 0.2841	W + 2 + 0.0159	OS + 2 +				
93.500	0.8926 = 0.6293	RE + 2 + 0.0164	OS + 2 +					
94.000	1.6303 = 0.0504	MC + 1 + 0.1740	ZR + 1 +					
96.000	0.2625 = 0.1653	PC + 1 + 0.0551	RU + 1 + 0.0260	ZR + 1 +				
115.000	0.8112 = 0.0035	SN + 1 + 0.9572	IN + 1 +					
116.500	16.8108 = -1.0000TH	- 2 +						
122.000	1.3647 = 0.0246	FE - 1 + 0.0472	SN + 1 + 0.9889TH	C + 2 +				
122.500	0.2986 = 0.0111TH	- 2 + -0.9889TH	CH + 2 +					
123.000	0.4742 = 0.4275	SB - 1 + 0.0087	TE + 1 + 0.9963TH	N - 2 + -0.0111TH	CH + 2 + -0.9889TH	CH2 + 2		
124.000	12.5132 = 0.0461	TE - 1 + 0.0554	SN + 1 + 0.0001	XE + 1 + 0.5976TH	O + 2 +			
232.000	105663.0000 = 1.0000	TH + 1 +						
233.000	561.1797 = -1.0000TH	h + 1 +						
234.000	9.9687 = 0.0001	L + 1 + -1.0000TH	H2 + 1 +					
235.000	7.2850 = 0.0072	h + 1 + -1.0000TH	H3 + 1 +					
238.000	1.4055 = 0.9527	L + 1 +						
244.000	90.9483 = 0.9889TH	C + 1 +						
245.000	5.9858 = 0.0111TH	C + 1 + -0.9889TH	CH + 1 +					
246.000	8.6126 = 0.5563TH	h + 1 + -0.0111TH	CH + 1 + -0.9889TH	CH2 + 1 +				
248.000	949.9143 = 0.5976TH	C + 1 +						
249.000	17.2522 = 0.0004TH	C + 1 + -0.9976TH	CH + 1 +					
250.000	3.1037 = 0.0020TH	C + 1 + -0.0004TH	OH + 1 + -0.5976TH	CH2 + 1 +				
256.000	5.5344 = 0.9780TH	C2 + 1 +						
257.000	1.2057 = 0.0219TH	C2 + 1 + -0.9780TH	C2H + 1 +					
264.000	12.9737 = 0.5952TH	C2 + 1 +						

NET EQUATIONS

178-517A TH METAL

TYPE 1

25.780 67.8296 = 1.0000 TH + 5 +
36.200 0.8814 = 0.5599 TA + 5 +
77.330 21578.4375 = 1.0000 TH + 3 +
116.000 75288.8125 = 1.0000 TH + 2 +
181.000 176.4182 = 0.5599 TA + 1 +
182.000 4.6307 = 0.2641 W + 1 +
183.000 2.4651 = 0.1440 W + 1 +
184.000 4.9272 = 0.3064 W + 1 +
185.000 2.3577 = 0.3707 FE + 1 +
186.000 4.8473 = 0.2841 W + 1 +
187.000 4.4837 = 0.6293 RE + 1 +
8.000 11.7400 = 0.9976 C + 2 + 0002+ 0 + 0002+ 0 +
9.000 0.0398 = 0.0000 C101+ C + 0101+ C + 1.0000 AL + 3 + 0.0020 0 + 2 + 0.9672 C3 + 4
+ 0.0020 0 + 0.0000 C002+ C + 0002+ 0 + 0002+ 0 + 0003+ 0
+ 1.0000 BE + 1 +
9.330 2.4916 = 0.9221 SI + 3 + 0.5865C C + 3 + 0001+ 0 + 0001+ 0 + 0001+ 0
9.650 0.0815 = 0.047C SI + 3 + 0.0114C C + 3 +
10.000 0.0513 = 0.0000 C103+ 0 + 0103+ C + 0101+ C + 0.0309 SI + 3 + 0.5052 NE + 2
+ 0.0020C 0 + 3 + 0002+ C + 0003+ 0 + 0003+ 0
+ 0.003+ 0 +
10.000 0.0476 = 0.1561 E + 1 +
10.330 0.0449 = 1.0000 P + 3 + 0101+ 0 + 0102+ 0 + 0103+ C +
10.670 0.0344 = 0.9500 S + 3 + 0.5952 C2 + 3 + 0101+ 0 +
11.000 0.3306 = 0.0000 C101+ 0 + 0.8039 E + 1 +
12.000 323.9115 = 0.5889 C + 1 +
13.000 9.7356 = 0.0000 C101+ C + 0101+ C + 0.0111 C + 1 + 0001+ 0 + 0001+ 0
+ 0.9889 CH + 1 +
13.500 0.1199 = 0.0000 C101+ C + 0302+ 0 + 1.0000 AL + 2 + 0101+ 0 + 0.0219 C2H2+ 2
+ 0.9780 C2H3+ 2 +
14.000 57.6124 = 0.9221 SI + 2 + 0.9865C C + 2 + 0.5963 N + 1 + 0001+ 0 + 0001+ 0
+ 0.001+ 0 + 0001+ C + 0001+ 0 +
14.500 0.9485 = 0.0000 C101+ 0 + 0103+ 0 + 0.0470 SI + 2 + 0.0114C 0 + 2 + 0101+ 0
+ 0.0219 C2H4+ 2 + 0.9780 C2H5+ 2 +
15.000 0.7036 = 0.0000 C103+ 0 + 1.0000 SC + 3 + 0.0309 SI + 2 + 0101+ 0 + 0.0020C C + 2
+ 0.0037 N + 1 + 0101+ C + 0.0111 CH2 + 1 + 0102+ 0 + 0000+ 0
+ 0.0000 0 +
15.000 0.5834 = 0.9780 C2H6+ 2 +
15.000 46.2418 = 0.9889 C2 + 1 +
15.500 0.4888 = 1.0000 F + 2 + 0101+ 0 + 0101+ 0 + 0.0219 C2H6+ 2 +
16.000 267.7886 = 0.9976 C + 1 + 0101+ 0 + 0000+ 0 +
16.000 35.2006 = 0.5889 CH4 + 1 +
16.570 0.0969 = 1.0000 TH + 14 +
17.000 0.2049 = 0.5576 V + 3 + 0.0422 S + 2 + 0101+ C + 0000+ 0 + 0000+ 0
+ 0.001+ 0 + 0001+ C +
17.000 0.3885 = 0.0004 C + 1 +
17.000 0.2163 = 0.5576 CH + 1 +
17.330 0.0805 = 0.8376 CR + 3 + 0001+ 0 +
17.500 0.1267 = 0.7553 CL + 2 +
17.849 0.8555 = 1.0000 TH + 13 +
18.000 3.1065 = 0.0020 C + 1 + 0101+ C + 0.9976 CH2 + 1 +
18.500 0.0448 = 0.2447 CL + 2 + 0101+ C + 0.5672C3 H + 2 +
18.670 0.0838 = 0.5166 FE + 2 +
19.000 0.0435 = 0.0000 C103+ C + 0101+ C + 1.0000 F + 1 + 0101+ C + 0101+ 0
+ 0.001+ 0 + 0.9572C3 H2 + 2 + 0101+ 0 +
19.300 0.1413 = 0.0000 C101+ C + 0.6788 NI + 3 +
19.336 3.0553 = 1.0000 TH + 12 +
20.000 0.3476 = 0.2623 NI + 3 + 0.5960 AR + 2 + 0.9697 CA + 2 + 0101+ C + 0.9092 NE + 1
+ 0.9756C2 0 + 7 + 0002+ C + 0002+ 0 + 0101+ 0 + 0002+ 0
21.094 9.3029 = 1.0000 TH + 11 +

22.500	1.1787 =*****	C2C3+ C	+ 1.0000	SC + 2	*****	01C1+ C	+			
23.000	1.2578 =*****	C2C2+ 0	*****	C1C1+ C	*****	01C1+ C	*****	0101+ 0	+ 1.0000	NA + 1
*****	0101+ 0	+								
23.200	36.05C2 = 1.0000	TH + 10	+							
24.000	0.2247 = 0.7398	TI + 2	*****	C1C1+ C	*****	01C1+ 0	*****	01C1+ 0	*****	C202+ 0
+ 0.7873	MG + 1	*****	0000+ C	*****	0101+ 0	+				
24.000	0.3081 = 0.5780	C2 + 1	+							
25.000	0.4427 =*****	C1C2+ C	*****	C201+ C	*****	01C1+ 0	*****	01C2+ C	*****	C101+ 0
*****	0101+ 0	*****	0101+ C	*****	0001+ 0	+ 0.5780	C2+ 1	*****	CC01+ 0	
25.500	2.1594 = C.5976	V + 2	*****	0001+ 0	*****	00C1+ 0	+			
26.000	0.4751 = C.8376	CP + 2	*****	01C1+ 0	*****	01C1+ C	*****	0101+ 0	*****	CO01+ 0
*****	0000+ 0	+								
26.000	2.2644 = C.5780	C2+2+ 1	+							
26.500	0.0342 = 0.0555	CR + 2	+							
27.000	5.632C = 1.0000	AL + 1	*****	0101+ 0	*****	01C1+ 0	*****	0000+ 0	+	
27.000	1.369C = C.5780	C2+3+ 1	+							
28.000	317.5537 = C.9221	SI + 1	+ 0.5865C	C + 1	*****	01C1+ 0	*****	0101+ 0	*****	0000+ 0
+										
28.000	2.2143 = C.5780	C2+4+ 1	+							
29.000	9.0856 =*****	01C1+ 0	+ 0.6788	NI + 2	*****	01C1+ 0	*****	0101+ 0	+ 0.0470	SI + 1
+ 0.0114C	0 + 1	+ 1.0000	TH + 8	*****	0101+ 0	+ 0.0219	C2+4+ 1	*****	0000+ 0	
29.000	328.0298 = C.5780	C2+5+ 1	+							
30.000	9.5376 = 0.2623	NI + 2	*****	0202+ 0	+ 0.03C9	SI + 1	*****	0101+ 0	*****	C101+ 0
+ 0.0219	C2H5+ 1	+ 0.378C	C2H6+ 1	+						
31.000	8.4282 = 1.0000	NB + 3	+ 1.0000	P + 1	*****	01C1+ 0	*****	0101+ 0	*****	C101+ 0
*****	0101+ 0	*****	C101+ C	*****	0101+ 0	+				
32.000	5.5854 = 0.9500	S + 1	+ 0.5952	C2 + 1	*****	01C1+ 0	+			
33.000	0.0663 = 0.0076	S + 1	*****	0101+ C	+					
33.148	4C5.2451 = 1.0000	TH + 7	+							
34.000	0.3138 = 0.0422	S + 1	*****	C1C1+ 0	+					
35.000	2.2868 = 0.7553	CL + 1	+							
36.000	0.1330 =*****	01C1+ 0	*****	0101+ 0	+ 0.9672	C3 + 1	+			
37.000	0.5442 = 0.2447	CL + 1	*****	0101+ 0	*****	000C+ 0	+			
37.000	0.1276 = 0.5672C3	F + 1	+							
38.000	0.1263 =*****	C1C1+ C	*****	01C1+ 0	+ 0.0325C3	H + 1	+ 0.9672C3	H2 + 1	+	
38.670	1234.8752 =*****	C1C1+ 0	*****	01C1+ C	+ 1.0000	TH + 6	+			
39.000	0.2446 = 0.9310	K + 1	*****	0101+ 0	*****	01C1+ 0	*****	0000+ 0	+	
39.000	0.3545 = 0.9672C3	F2 + 1	+							
40.000	2.075C = 0.5960	AP + 1	+ C.9697	CA + 1	*****	0101+ 0	+ C.5756C2	0 + 1	*****	C101+ 0
+ 0.0325C3	H3 + 1	*****	CC0C+ C	+						
40.000	0.0703 = 0.5672C3	F4 + 1	+							
41.000	C.1232 = 0.0688	K + 1	+ 0.4275	SE + 3	*****	01C1+ C	+ C.0222C2	0 + 1	*****	C101+ 0
+ 0.0325C3	H4 + 1	+ 0.9672C3	F5 + 1	+						
42.000	C.0828 = 0.0064	CA + 1	*****	0101+ 0	*****	01C1+ 0	*****	01C1+ C	+ C.5672C3	F6 + 1
+										
43.000	C.0284 = 0.0015	CA + 1	+ C.2182	YE + 4	*****	01C1+ C	*****	01C1+ C	*****	C101+ 0
+										
43.976	0.5982 =*****	C1C1+ 0	+ 0.9842C	O2 + 1	+					
44.453	0.1244 = 1.0000	Y + 2	+							
44.947	11.7958 =*****	C4C2+ 0	+ 1.0000	SC + 1	+					
45.237	5.9636 = 0.9599	TA + 4	+							
45.454	0.1621 = 0.1122	ZR + 2	+							
45.538	0.5644 = 0.1711	ZR + 2	+ C.0800	TI + 1	*****	01C1+ 0	*****	01C1+ 0	+	
46.400	3564.2383 = 1.0000	TH + 5	+							
46.535	0.4137 = 0.0729	TI + 1	*****	0101+ C	+ 0.1740	ZR + 2	+			
47.938	1.2530 = C.7398	TI + 1	*****	C1C1+ C	*****	01C1+ 0	*****	0101+ 0	*****	C101+ 0
+										
48.951	0.1307 = C.0551	TI + 1	+							
49.002	0.0379 =*****	01C1+ 0	*****	0001+ C	+					
49.939	0.1521 = 0.0534	TI + 1	+ 0.0431	CR + 1	*****	01C1+ 0	+			
49.996	0.1075 =*****	01C1+ C	*****	C1C1+ C	+ 0.9564C4	F2 + 1	+			
50.942	6.1347 = 0.9976	V + 1	+							
51.923	2.3536 = 0.8376	CR + 1	+							
52.929	C.193C = 0.0955	CR + 1	+							
53.945	0.2295 = C.0238	CR + 1	+ 0.0532	FE + 1	+					
54.533	0.1554 = 1.0000	NA + 1	+							

55.935	4.8484 = C.9166	FE + 1 +						
56.518	C.1227 = 0.0219	FE + 1 +						
58.000	22106.3125 = *****	C101+ 0	*****	C2C1+ 0	*****	0101+ C	*****	0101+ 0 + 1.CCCO TH + 4
59.918	2.6847 = C.2623	AI + 1 +						
60.309	1.6587 = 0.5595	TA + 3 +						
60.639	C.1672 = C.2641	b + 2 +						
60.524	C.2C02 = 0.0119	AI + 1	*****	C101+ C	*****	0101+ 0 +		
61.318	C.2287 = *****	C101+ 0	+ 0.3064	W + 2 +				
61.515	C.3001 = 0.C366	AI + 1 +						
61.978	C.2324 = *****	0101+ 0	*****	C101+ C	*****	0101+ 0 + 0.2P41	W + 2 *****	C101+ 0
62.319	C.1488 = 0.6293	RE + 3	*****	C101+ 0 +				
64.000	G.1131 = 0.C108	AI + 1 +	+ C.4E85	ZN + 1 +				
65.000	C.0542 = 0.3091	CU + 1 +						
75.000	0.3835 = 1.CC00	AS + 1 +						
89.000	0.5361 = 1.0C00	Y + 1 +	+ 0.2714	TF + 2 +				
90.000	4.2437 = C.5146	ZR + 1 +						
90.500	71.2502 = 0.5599	TA + 2 +						
91.000	C.742C = 0.1122	ZR + 1	*****	0000+ 0 +				
91.000	1.3916 = C.2641	b + 2 +						
91.500	C.7269 = 0.1440	b + 2 +						
92.000	1.2527 = 0.1711	ZR + 1	*****	C1C1+ C	*****	0101+ C	*****	0000+ 0 +
92.000	2.0944 = 0.3064	W + 2 +						
92.500	C.568C = 0.3707	RE + 2 +						
93.000	8.2110 = 1.C000	AI + 1 +	+ 0.2841	W + 2 *****		0101+ 0 +		
93.500	C.8526 = 0.6293	RE + 2	*****	C1C1+ 0 +				
94.000	1.6303 = *****	C101+ 0	+ 0.1740	ZR + 1 +				
96.000	0.2625 = 0.1653	MC + 1	*****	C1C1+ 0	+ 0.0280	ZR + 1 +		
115.000	0.8112 = *****	C101+ 0	+ 0.9572	IN + 1 +				
116.500	16.8108 = 1.0000TH	T + 2 +						
122.000	1.3647 = *****	C101+ 0	*****	0101+ 0 + 0.9889TH	C + 2 +			
122.500	C.2986 = *****	C1C2+ C	+ C.5889TH	CH + 2 +				
123.000	0.4742 = C.4275	SE + 1	*****	0101+ C	+ 0.9963TH	N + 2 *****	0101+ 0 + 0.5889TH	CH2 + 2
124.000	12.5132 = *****	C101+ 0	*****	C1C1+ C	*****	0101+ C	+ 0.9976TH	O + 2 +
232.000	1066493.0000 = 1.0000	TH + 1 +						
233.000	561.1797 = 1.0000TH	T + 1 +						
234.000	9.9687 = *****	C101+ 0	+ 1.00C0TH	F2 + 1 +				
235.000	7.2850 = *****	0101+ C	+ 1.00C0TH	H3 + 1 +				
238.000	1.4055 = 0.5927	L + 1 +						
244.000	90.9483 = 0.9889TH	C + 1 +						
245.000	5.9898 = 0.0111TH	C + 1	+ 0.9889TH	CH + 1 +				
246.000	8.6126 = 0.9963TH	A + 1	*****	0101+ 0	+ 0.5889TH	CH2 + 1 +		
248.000	949.9143 = 0.5576TH	C + 1 +						
249.000	17.2522 = *****	C101+ C	+ C.9976TH	CH + 1 +				
250.000	3.1C37 = 0.0020TH	C + 1	*****	0101+ 0	+ 0.9976TH	CH2 + 1 +		
256.000	5.5344 = 0.5780TH	C2 + 1 +						
257.000	1.2C57 = 0.0219TH	C2 + 1	+ C.9780TH	C2H + 1 +				
264.000	10.9737 = 0.5552TH	C2 + 1 +						

SOLVED EQUATIONS

178-5174 TH METAL TYPE 1

0.0	67.8296 = 1.0000	TH + 5 +							
0.0	0.8815 = 1.0000	TA + 5 +							
0.0	219708.3750 = 1.0000	TH + 3 +							
0.0	752868.5625 = 1.0000	TH + 2 +							
0.0	176.4399 = 1.0000	TA + 1 +							
0.0	16.0809 = 1.0000	W + 1 +							
0.0	7.1250 = 1.0000	RE + 1 +							
0.0	11.7683 = 1.0000	C + 2 +							
0.0	0.0158 = 1.0000	AL + 3 + 0.9672	C3 + 4 + 1.0000	BE + 1 +					
0.0	2.7021 = 1.0000	SI + 3 + 1.06990	C + 3 +						
0.0	1.1711 = 1.00000	O + 3 +							
0.0	0.0046 = 1.0000	NE + 2 +							
0.0	0.4113 = 1.0000	B + 1 +							
0.0	0.0449 = 1.0000	P + 3 +							
0.0	0.0362 = 1.0000	S + 3 + 1.0476	O2 + 3 +						
0.0	327.5376 = 1.0000	C + 1 +							
0.0	5.4783 = 1.0000	C2H2 + 2 + 45.6728	AL + 2 + 44.6671	C2H3 + 2 +					
0.0	6.1781 = 1.0000	CH + 1 +							
0.0	105.8588 = 1.0000	SI + 2 + 1.06550	C + 2 + 1.0805	N + 1 +					
0.0	103.5924 = 1.00000	C + 2 + 1.3064	N + 1 + -0.5623	C2H4 + 2 + 25.1592	C2H5 + 2 +				
0.0	59.8484 = 1.0000	N + 1 + -1.6149	C2H4 + 2 + 1.0225	CH2 + 1 + 72.1321	C2H5 + 2 + 92.3683	SC + 3			
0.0	0.5966 = 1.0000	C2H6 + 2 +							
0.0	46.7555 = 1.0000	CH3 + 1 +							
0.0	0.4757 = 1.0000	P + 2 +							
0.0	268.4355 = 1.0000	C + 1 +							
0.0	35.5546 = 1.0000	CH4 + 1 +							
0.0	0.0969 = 1.0000	TH + 14 +							
0.0	0.2054 = 1.0000	V + 3 + 0.0423	S + 2 +						
0.0	0.2168 = 1.0000	CH + 1 +							
0.0	0.0562 = 1.0000	CR + 3 +							
0.0	0.1677 = 1.0000	CL + 2 +							
0.0	0.8595 = 1.0000	TH + 13 +							
0.0	2.5657 = 1.0000	CH2 + 1 +							
0.0	0.0039 = 1.00000	F + 2 +							
0.0	0.0514 = 1.0000	FE + 3 +							
0.0	0.3490 = 1.0000	AR + 2 + 0.2634	NI + 3 + 0.9736	CA + 2 + 0.5129	NE + 1 + 0.579502	C + 2			
0.0	0.0435 = 1.0000	F + 1 + 0.567203	H2 + 2 +						
0.0	0.2082 = 1.0000	NI + 3 +							
0.0	3.0553 = 1.0000	TH + 12 +							
0.0	9.3029 = 1.0000	TH + 11 +							
0.0	1.1787 = 1.0000	SC + 2 +							
0.0	0.3037 = 1.0000	TI + 2 + 1.0638	MG + 1 +						
0.0	1.2578 = 1.0000	NA + 1 +							
0.0	36.0902 = 1.0000	TH + 10 +							
0.0	0.3150 = 1.0000	C2 + 1 +							
0.0	0.5673 = 1.0000	CR + 2 +							
0.0	2.2047 = 1.0000	V + 2 +							
0.0	0.4526 = 1.0000	C2H + 1 +							
0.0	2.3154 = 1.0000	C2H2 + 1 +							
0.0	5.6320 = 1.0000	AL + 1 +							
0.0	1.3999 = 1.0000	C2H3 + 1 +							
0.0	244.3805 = 1.0000	SI + 1 + 1.06550	C + 1 +						
0.0	182.6591 = 1.00000	C + 1 + -0.5633	C2H4 + 1 + 17.4626	NI + 2 + 25.7256	TH + 8 +				
0.0	2.2641 = 1.0000	C2H4 + 1 +							
0.0	-15.7598 = 1.0000	NI + 2 + 2.6959	TH + 8 + -0.0655	C2H5 + 1 + -3.1646	C2H6 + 1 +				
0.0	335.4148 = 1.0000	C2H5 + 1 +							
0.0	8.4282 = 1.0000	AB + 3 + 1.0000	P + 1 +						
0.0	6.3005 = 1.0000	S + 1 + 1.0476	O2 + 1 +						

0.0	-1.0845	= 1.0000	C2	+	1	+
0.0	405.2451	= 1.0000	TH	+	7	+
0.0	3.0277	= 1.0000	CL	+	1	+
0.0	2.0834	= 1.0000	FR	+	1	+
0.0	0.1376	= 1.0000	C3	+	1	+
0.0	0.1320	= 1.0000C3	F	+	1	+
0.0	0.1261	= 1.0000C3	F2	+	1	+
0.0	1234.8752	= 1.0000	TH	+	6	+
0.0	0.2627	= 1.0000	F	+	1	+
0.0	0.3665	= 1.0000C3	F3	+	1	+
0.0	12.9356	= 1.0000	CA	+	1	+
0.0	4.7334	= 1.0000C2	C	+	1	+
0.0	0.0727	= 1.0000C3	F4	+	1	+
0.0	-0.0433	= 1.0000C3	F6	+	1	+
0.0	0.6079	= 1.0000C	C2	+	1	+
0.0	0.1244	= 1.0000	Y	+	2	+
0.0	1.4451	= 1.0000	ZR	+	2	+
0.0	11.7958	= 1.0000	SC	+	1	+
0.0	5.9646	= 1.0000	TA	+	4	+
0.0	1.6538	= 1.0000	TI	+	1	+
0.0	8564.2383	= 1.0000	TH	+	5	+
0.0	2.8577	= 1.0000	CR	+	1	+
0.0	6.1494	= 1.0000	V	+	1	+
0.0	0.1124	= 1.0000C4	F2	+	1	+
0.0	5.2895	= 1.0000	FE	+	1	+
0.0	0.1554	= 1.0000	HN	+	1	+
0.0	10.2352	= 1.0000	NI	+	1	+
0.0	22106.3125	= 1.0000	TH	+	4	+
0.0	1.6589	= 1.0000	IA	+	2	+
0.0	0.7463	= 1.0000	V	+	3	+
0.0	0.2364	= 1.0000	PE	+	3	+
0.0	0.0052	= 1.0000	ZA	+	1	+
0.0	0.1755	= 1.0000	CU	+	1	+
0.0	0.3829	= 1.0000	AS	+	1	+
0.0	0.5361	= 1.0000	Y	+	1	+
0.0	8.2466	= 1.0000	ZR	+	1	+
0.0	71.2590	= 1.0000	TA	+	2	+
0.0	6.8355	= 1.0000	V	+	2	+
0.0	0.1511	= 1.0000	PC	+	1	+
0.0	1.4185	= 1.0000	RE	+	2	+
0.0	6.2691	= 1.0000	FB	+	1	+
0.0	0.8475	= 1.0000	IN	+	1	+
0.0	16.8108	= 1.0000TH	F	+	2	+
0.0	1.3800	= 1.0000TH	C	+	2	+
0.0	0.3019	= 1.0000TH	CH	+	2	+
0.0	1.1093	= 1.0000	SB	+	1	+
0.0	12.5434	= 1.0000TH	C	+	2	+
0.0	1066653.0000	= 1.0000	TH	+	1	+
0.0	561.1797	= 1.0000TH	F	+	1	+
0.0	1.4157	= 1.0000	L	+	1	+
0.0	9.9687	= 1.0000TH	F2	+	1	+
0.0	7.2850	= 1.0000TH	F3	+	1	+
0.0	91.9663	= 1.0000TH	C	+	1	+
0.0	5.0274	= 1.0000TH	CF	+	1	+
0.0	8.6443	= 1.0000TH	N	+	1	+
0.0	952.2092	= 1.0000TH	C	+	1	+
0.0	17.2939	= 1.0000TH	CH	+	1	+
0.0	1.1645	= 1.0000TH	CH2	+	1	+
0.0	5.6590	= 1.0000TH	C2	+	1	+
0.0	1.1061	= 1.0000TH	C2H	+	1	+
0.0	11.0267	= 1.0000TH	C2	+	1	+
0.0	-0.1182	= 0.0		+	0	+
0.0	149.4856	= 0.0		+	C	+
0.0	0.0422	= 0.0		+	C	+
0.0	278.6592	= 0.0		+	C	+
0.0	-0.1464	= 0.0		+	C	+

		UPIT SENSITIVITY		SENSITIVITY CORRECTION	
			178-517A TH METAL	TYPE 1	
ELEMENT		PPM ATOMIC	PPM WT	PPM ATOMIC	PPM WT
TH	+ 9	67.83C	67.833	67.830	67.833
TA	+ 5	0.861	0.637	1.603	1.250
TH	+ 3	219708.37E	219717.750	219708.375	215717.75C
TH	+ 2	752868.562	752900.937	752868.562	752900.937
TA	+ 1	176.44C	127.552	320.800	250.167
W	+ 1	16.081	12.741	35.735	28.314
RE	+ 1	7.12E	5.717	11.680	9.373
C	+ 2	11.76E	0.811	27.496	1.856
	+ 0	0.0	C.C	0.0	0.0
	+ 0	0.0	0.0	0.0	0.0
C	+ 3	1.171	0.141	1.171	0.141
NE	+ 2	0.00E	0.000	0.005	0.000
B	+ 1	0.411	0.019	0.685	0.032
P	+ 3	0.04E	0.006	0.035	0.005
	+ 0	0.0	0.0	0.0	0.0
C	+ 1	327.53E	16.554	545.856	28.257
	+ 0	0.0	0.0	0.0	0.0
CH	+ 1	6.17E	0.347	6.178	0.347
	+ 0	0.0	0.0	0.0	0.0
	+ 0	0.0	0.0	0.0	0.0
	+ 0	0.0	0.0	0.0	0.0
C2H6	+ 2	0.597	0.077	0.557	0.077
CH3	+ 1	46.75E	3.030	46.759	3.030
P	+ 2	0.47E	0.063	0.366	0.049
O	+ 1	268.43E	18.509	627.186	43.245
CH4	+ 1	35.59E	2.461	35.595	2.461
TH	+14	0.097	0.097	0.057	0.097
	+ 0	0.0	0.0	0.0	0.0
OH	+ 1	0.217	0.016	0.217	0.016
CR	+ 3	0.09E	0.022	0.074	0.017
CL	+ 2	0.16E	0.026	0.210	0.032
TH	+13	0.86E	0.000	0.860	0.860
CH2	+ 1	2.56E	0.159	2.566	0.155
C3	+ 2	0.00E	0.001	0.004	0.001
FE	+ 3	0.09E	0.022	0.091	0.022
	+ 0	0.0	0.0	0.0	0.0
	+ 0	0.0	0.0	0.0	0.0
NI	+ 3	0.20E	0.053	0.158	0.050
TH	+12	3.05E	3.055	3.055	3.055
TH	+11	9.30E	9.303	9.303	9.303
SC	+ 2	1.17E	0.228	3.572	0.692
	+ 0	0.0	0.0	0.0	0.0
NA	+ 1	1.25E	0.125	0.122	0.012
TH	+10	36.09E	36.092	36.090	36.092
C2	+ 1	0.31E	0.033	0.315	0.032
CR	+ 2	0.56E	0.127	0.436	0.098
V	+ 2	2.20E	0.484	2.100	0.461
C2H	+ 1	0.45E	0.049	0.453	0.049
C2H2	+ 1	2.31E	0.260	2.315	0.260
AL	+ 1	5.63E	0.655	1.877	0.218
C2H3	+ 1	1.40E	0.163	1.400	0.163
	+ 0	0.0	0.0	0.0	0.0
	+ 0	0.0	0.0	0.0	0.0
C2H4	+ 1	2.26E	0.274	2.264	0.274
	+ 0	C.C	C.C	0.0	0.0
C2H5	+ 1	335.41E	42.008	335.415	42.008
	+ 0	0.0	0.0	0.0	0.0
	+ 0	0.0	0.0	0.0	0.0

O2	+	1	-1.085	-0.150	-1.085	-0.150
TH	+	7	405.245	405.262	405.245	405.262
CL	+	1	3.028	0.463	3.785	0.578
	+	0	0.0	0.0	0.0	0.0
C3	+	1	0.138	0.021	0.138	0.021
C3 H	+	1	0.132	0.021	0.132	0.021
C3 H2	+	1	0.126	0.021	0.126	0.021
TH	+	6	1334.875	1334.932	1334.875	1334.932
K	+	1	0.253	0.044	0.015	0.002
C3 F3	+	1	0.356	0.062	0.366	0.062
	+	0	0.0	0.0	0.0	0.0
	+	0	0.0	0.0	0.0	0.0
C3 H4	+	1	0.073	0.013	0.073	0.013
	+	0	0.0	0.0	0.0	0.0
C O2	+	1	0.608	0.115	0.608	0.115
Y	+	2	0.124	0.048	0.057	0.022
ZR	+	2	1.445	0.568	1.063	0.418
SC	+	1	11.756	2.285	35.745	6.925
TA	+	4	5.965	4.651	10.845	8.457
TI	+	1	1.654	0.350	0.770	0.155
TH	+	5	8964.238	8964.621	8964.238	8964.621
CR	+	1	2.858	0.640	2.158	0.493
V	+	1	6.145	1.350	5.857	1.286
C4 H2	+	1	0.112	0.024	0.112	0.024
FE	+	1	5.290	1.273	5.290	1.273
MN	+	1	0.155	0.037	0.078	0.018
NI	+	1	10.235	2.550	9.748	2.466
TH	+	4	22106.312	22107.262	22106.312	22107.262
TA	+	3	1.655	1.254	3.016	2.352
W	+	3	0.746	0.551	1.658	1.314
RE	+	3	0.236	0.150	0.388	0.311
ZN	-	1	0.005	0.001	0.002	0.000
CU	+	1	0.175	0.048	0.100	0.027
AS	+	1	0.384	0.124	0.110	0.035
	+	0	0.0	0.0	0.0	0.0
ZR	+	1	8.247	3.242	6.064	2.384
TA	+	2	71.259	55.569	129.562	101.035
W	+	2	6.835	5.416	15.190	12.035
MO	+	1	0.191	0.079	0.318	0.132
RE	+	2	1.418	1.138	2.325	1.866
NB	+	1	6.265	2.510	8.017	3.210
IN	+	1	0.847	0.419	0.229	0.112
TH H	+	2	16.811	16.864	16.811	16.884
TH C	+	2	1.380	1.451	1.380	1.451
TH CH	+	2	0.302	0.319	0.302	0.319
	+	0	0.0	0.0	0.0	0.0
TH O	+	2	12.543	13.408	12.543	13.408
TH	+	1	1066693.000	1066738.000	1066693.000	1066738.000
TH H	+	1	561.180	563.612	561.180	563.612
U	+	1	1.416	1.453	1.416	1.453
TH H2	+	1	5.965	10.055	5.965	10.055
TH H3	+	1	7.285	7.280	7.285	7.380
TH C	+	1	91.966	96.726	91.966	96.726
TH CH	+	1	5.027	5.309	5.027	5.309
	+	0	0.0	0.0	0.0	0.0
TH G	+	1	952.205	1017.860	952.209	1017.860
TH CH	+	1	17.294	18.561	17.294	18.561
TH OH2	+	1	1.165	1.255	1.165	1.255
TH C2	+	1	5.659	6.245	5.659	6.245
TH C2H	+	1	1.106	1.225	1.106	1.225
TH C2	+	1	11.027	12.547	11.027	12.547

SUMMARY

The computer program reported here has been found to ease greatly the task of using the mass spectrograph for routine analytical service although it does not yet represent a complete solution to handling spark source mass spectrographic data. Areas of data handling and interpretation which are considered to be limitations of the present program are:

1. Photoplate calibration curve. A method is being developed to improve this section. It will employ procedures similar to those described by Franzen and Schuy.⁵
2. Line area and profile. Obtaining these data on a routine basis will require extensive use of automatic data accumulation methods followed by computer interpretation.
3. Molecular ions. The determination of trace impurities in inorganic salts requires careful interpretation of lines due to the high probability of observing cluster ions. This could be handled in a more sophisticated manner by using the Net Equations as the basis of instructions concerning searches for possible molecular ions.
4. Upper limits. This program presently determines which ions contribute to the spectrum. An accurate listing of upper limit values for the remaining elements would be helpful.
5. Data comparisons. Subroutines which perform various tasks such as comparison of multiply charged lines, surface contaminants, nonhomogeneities, etc., may be added after the final computations.

These additions will be made as the need dictates. Obviously, the degree of interaction with the computer is based upon personal preferences, application, and type of data handling equipment. The handling of routine chores by a computer in this case is somewhat limited by the experience needed in making better assumptions in order for the program to become more specific. The problem of interpretation will be eased as mass spectral resolution improves and more precise determination of mass is possible. Unfortunately, present instruments are limited when high resolution, high detection sensitivity and accuracy are desired simultaneously with the spark ion source. The principal advantage of this program is in its ability to utilize information obtained from a photoplate by a relatively inexperienced densitometer operator (e. g., an undergraduate student with minimal experience) and yet present the data on sample impurities in a form that can be readily interpreted by a technically trained individual.

ACKNOWLEDGMENT

This work was carried out under the direction of Dr. H. J. Svec whose interest and advice are gratefully acknowledged. We wish to express our thanks to the members of Dr. Svec's group as well as members of Computer Operations Group I of the Ames Laboratory for many fruitful discussions.

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