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COMPUTER PROGRAMS FOR THE INTERPRETATION OF LOW RESOLUTION MASS SPECTRA: PROGRAM FOR CALCULATION OF MOLECULAR ISOTOPIC DISTRIBUTION AND PROGRAM FOR ASSIGNMENT OF MOLECULAR FORMULAS

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16. Abstract

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COMPUTER PROGRAMS FOR THE INTERPRETATION OF LOW RESOLUTION MASS SPECTRA: PROGRAM FOR CALCULATION OF MOLECULAR ISOTOPIC DISTRIBUTION AND PROGRAM FOR ASSIGNMENT OF MOLECULAR FORMULAS

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SUMMARY

Two FORTRAN computer programs for the interpretation of low resolution mass spectra have been prepared and tested. One is for the calculation of the molecular isotopic distribution of any species from stored elemental distributions. The program requires only the input of the molecular formula and has been designed to be compatable with any computer system. The other program is for the determination of all possible combinations of atoms (and radicals) which may form an ion having a particular integer mass. It also uses a simplified input scheme and has been designed to be compatable with any system.

INTRODUCTION

The mass spectroscopist is faced with several laborious tasks when he is attempting to identify an ion from its mass and isotopic distribution. One task is to select all ions which may give rise to a particular mass. Another is to calculate the relative molecular isotopic abundances of these ions for comparison with the experimental distribution. Two new computer programs which may be used for these tasks are described here. These programs are easier to handle and more encompassing than previous methods and computer programs (refs. 1 and 2). The ease of use of our pro-

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grams arises from having all necessary atomic data contained within the program. Moreover, the programs are easily adaptable to most computer systems.

CALCULATION OF MOLECULAR ISOTOPIC DISTRIBUTIONS

Grimley (ref. 3) has presented an algorithm which may be used to obtain molecular isotopic distributions from known elemental distributions. With this method, two elemental distributions are first combined. The resulting diatomic distribution is then combined with another elemental distribution to construct a triatomic distribution. This process is repeated until the distribution for the desired ionic species is obtained. This method, although tractable for hand-calculations of small ions, becomes very tedious for larger species.

For multiatomic species high-speed computer techniques are most convenient. For this reason we have prepared a computer program which may be used to calculate these distributions. In order to encourage the use of this program over hand calculations, thereby avoiding the associated error and tedium, a simplified input scheme is used. The only input required is the molecular formula; all other information is stored permanently within the program. For example, the distribution for the molybdenum trioxide trimer molecule $(MoO_3)_3$, would be obtained after entering MO 3 O 9.

The output of this program is shown in figure 1(a). It consists of the molecular formula, the individual elemental distributions, and the molecular distribution. This molecular distribution is displayed both numerically and graphically; the latter display is especially useful for rapid comparisons of experimental and calculated distributions. The run time for this calculation was 1.2 seconds on the IBM 360. A second example, for dibromochlorotrifluorobutane, $C_4H_4Br_2ClF_3$, is given in figure 1(b).

The few other programs available for this type of calculation (refs. 1 and 2) all have limitations. Of the three programs given in these references, one is limited to a few atoms; another requires the input of atomic distributions for each atom in the molecule; and the remaining program requires the input of a complete table of distributions with each run. Furthermore, all require the input of additional data such as the atomic numbers and the number of atoms.

A listing of our program is given in appendix A. This program has run successfully on the UNIVAC 1110 system at Lewis Research Center and, with a few modifications, on the IBM 360 system. This program is called DISMIS for distribution of molecular isotopes. It is coded in standard FORTRAN IV and can be readily adapted to both time-sharing and batch-processing systems. Moreover, its output can be easily changed from the 129-column form to a 79-column form for teletypes. The required modifications are given in comment cards located within program listing. The ele-

mental isotopic distributions of all stable elements are contained in a subroutine called DISEIS. These data were taken from a recent tabulation by Roboz (ref. 4).

The program is set up to accept molecules having up to 10 different atomic species. The molecular formula, which is the only input required, is entered in 10(A2, I2) format. The common symbols for the elements are used, and those symbols and subscripts having a single character must be preceded by a blank space. Sufficient memory has been set aside within the program to calculate the distribution for virtually any molecule which can be detected mass spectrometrically.

ASSIGNMENT OF MOLECULAR FORMULAS

The technique described here can be used to prepare a list of those species, possibly present in a system, which have a specified mass number. For example, in figure 2(a) all possible combinations of K, Cl, Cr, and O atoms which have a mass number of 294 have been determined. From this list one may choose those species which are intuitively reasonable, and then further analyze them using the isotopic distribution program. For the example in figure 2(a) the best candidate was the potassium dichromate ion, $K_2Cr_2O_7^+$. The run time required for this calculation was 1.2 seconds on the IBM 360. A second example is shown in figure 2(b), where the most reasonable choice for the mass to charge ratio m/e 118 was $CrO_2(OH)_2^+$.

There have been a few tabulations of molecular formulas as a function of mass (refs. 5 and 6), but these are limited to four and 16 elements, respectively. There are also a few computer programs available (e.g., refs. 7 and 8). However, of the three programs listed in these references, two are designed for high resolution, generally organic, spectra, and the third is written in BASIC. All are limited to a few atoms.

A listing of our program, including pertinent COMMENT cards for the conversion from batch processing to time sharing computer systems, is given in appendix B. This version has run on the IBM 360. The mass number of the most abundant isotope for 57 elements have been included in the program. These represent all of the stable elements for which this isotope accounts for at least 60 percent of the total. Thus, elements such as platinum have been excluded. In addition to the elements contained in this program, the radicals OH, H_2O, and CH_3 have also been included. Up to 12 more radicals may be added to the array ATOM by replacing two of the present zeroes with a two-digit symbol and the mass number, respectively. More radicals may be added if the dimension is increased.

The input to the program consists of the symbols of up to nine of the stored atoms or radicals entered in 9A2 format. This is followed by the value of m/e under consideration. It is entered in I4 format and must be right justified; for example, a two-

digit number must be preceded by two blank spaces. One then enters the maximum number of each atom to be considered. This is mandatory with the batch processing program; however, with the time sharing program, upper limits for these values will be calculated and then lower values may be added if desired.

As seen before, the output of the program consists of a listing of all possible combinations of the entered atoms which have a specified mass. Because these molecular masses are based on the masses of the most abundant atomic isotope, errors can occur if those atomic isotopes do not account for most of the intensity. This is especially true when several of the same atoms are being considered. For example, for the ion $K_4Cl_3^+$, the atoms ^{39}K and ^{35}Cl account for about 93 and 75 percent of the total, respectively. For this ion the most abundant mass is not 261 atomic mass units (amu) as one may have expected but instead 263 amu. Thus, one must always consider the full distribution, as calculated using the program DISMIS, before assigning an ion to a mass number.

The user of this program may also wish to limit both the number of different atoms to be considered and the maximum number of each. Such restrictions, when made carefully, can often result in substantial savings of computer time without missing any reasonable species. However, the user must severely restrict the number of hydrogen atoms to be considered. If this is not done, the number of species having the molecular mass of interest would be prohibitive. Thus, the program is especially useful for inorganic species where the number of hydrogen atoms in a molecule is generally less than for organics. Indeed, we have used the program to interpret the low resolution spectra of inorganic systems and have found it to be an invaluable aid for recognizing all possible species which may be in a system.

The program is called FINDME which stands for: find m/e. As with the previously described program it has been designed for ease of use, compatability with other FORTRAN IV compilers, use with batch processing or time sharing systems, and use with any output device having, in this case, at least 52 columns.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, April 28, 1977,
506-16.

APPENDIX A

LISTING OF COMPUTER PROGRAM FOR THE CALCULATION OF MOLECULAR ISOTOPIC DISTRIBUTIONS

```
      DIMENSION AT(10),NAT(10),ATM(100)
C     FOR TTY CHANGE TO  PLOT(50)
      DIMENSION A1(500),A2(10),FRC(500),PLOT(100)
      DATA DASH,BLANK,PLUS/'-',' ','+'/
C     FOR TIME SHARING SYSTEMS REMOVE THE FOLLOWING 'C'
C     WRITE(6,500)
500   FORMAT('0ENTER MOLECULE IN 10(A2,I2) FORMAT; RIGHT JUSTIFY')
50    READ(5,100,END=51) (AT(I),NAT(I),I=1,10)
100   FORMAT(10(A2,I2))
      NIS=10
      NA=0
      DO 1 I=1,NIS
      J=NAT(I)
      IF(J.EQ.0) GOTO 1
      ITOP=I
      DO 2 II=1,J
      NA=NA+1
      ATM(NA)=AT(I)
2     CONTINUE
1     CONTINUE
      WRITE(6,101) (AT(I),NAT(I),I=1,ITOP)
101   FORMAT(///'1 ISOTOPIC DISTRIBUTION FOR     '10(A2,I2))
      WRITE(6,102)
102   FORMAT('0 ELEMENTAL DISTRIBUTIONS')
      CALL DISEIS(ATM(1),L1,A1,SUM,NSI)
      LH=L1+NSI-1
      LE=LH
      IF(NSI.GT.7) LE=L1+6
      WRITE(6,103) ATM(1),(M,M=L1,LE)
      NISO=NSI
      IF(NSI.GT.7) NISO=7
      WRITE(6,107) (A1(I),I=1,NISO)
      IF(NSI.LE.7) GOTO 20
      LE=LE+1
      WRITE(6,108) (M,M=LE,LH)
      WRITE(6,107) (A1(I),I=8,NSI)
20    IF((SUM.GT.1.0005).OR.(SUM.LT..9995)) WRITE(6,109) SUM
103   FORMAT(A7,I3,6I11)
107   FORMAT(7X,7F11.6)
108   FORMAT(7X,I3,6I11)
109   FORMAT(9X,'  NOTE  SUM ='F9.6)
      NSI=NIS
      ZERO=1.E-8
      DO 3 IA=2,NA
      CALL DISEIS(ATM(IA),L2,A2,SUM,NIS)
      IF(ATM(IA).EQ.ATM(1)) GOTO 21
      LH=L2+NIS-1
```

```
      LE=LH
      IF(NIS.GT.7) LE=L2+6
      WRITE(6,103) ATM(IA),(M,M=L2,LE)
      NISO=NIS
      IF(NIS.GT.7) NISO=7
      WRITE(6,107) (A2(I),I=1,NISO)
      IF(NIS.LE.7) GOTO 22
      LE=LE+1
      WRITE(6,108) (M,M=LE,LH)
      WRITE(6,107) (A2(I),I=8,NIS)
22    IF((SUM.GT.1.0001).OR.(SUM.LT..9999)) WRITE(6,109) SUM
21    CONTINUE
      ATM(1)=ATM(IA)
      L1=L1+L2
      NI=NSI+NIS-1
      DO 4 NMI=1,NI
      N=NMI+1
      NMT=NMI
      IF(NMT.GT.NSI) NMT=NSI
      NS=N-NIS
      IF(NS.LE.0) NS=1
      FRAC=0.
      DO 5 I1=NS,NMT
      I2=N-I1
      FRAC=A1(I1)*A2(I2)+FRAC
5     CONTINUE
      FRC(NMI)=FRAC
      IF(FRAC.LT.ZERO) FRC(NMI)=0.
      IF(FRAC.GT.ZERO) NSS=NMI
4     CONTINUE
      NSI=NSS
      DO 6 II=1,NSI
      A1(II)=FRC(II)
6     CONTINUE
3     CONTINUE
      NIMIN=0
      NIMAX=NSI
      SUMM=0.
      FRCMAX=0.
      DO 7 I=1,NSI
      F=FRC(I)
      IF(F.GT.FRCMAX) FRCMAX=F
      IF(F.GT.ZERO) NIMAX=I
      SUMM=F+SUMM
      IF(NIMIN.GT.0) GOTO 7
      IF(F.GT.ZERO) NIMIN=I
7     CONTINUE
C     FOR TTY CHANGE TO  NPLOT=50
      NPLOT=100
      IPLT=NPLOT/10
      WRITE(6,104) (I,I=1,10)
104   FORMAT('0 MOLECULAR DISTRIBUTION',/,-
C     FOR TTY CHANGE TO  10I5
     & '    M/E    ABSOLUTE    RELATIVE   ',10I10)
      DO 8 I=NIMIN,NIMAX
      F=FRC(I)
      MASS=L1+I-1
```

```
      RELFRC=F/FRCMAX
      IF(RELFRC.LT..005) GOTO 19
      DO 9 J=1,NPLOT
9     PLOT(J)=BLANK
      N=RELFRC*NPLOT+.5
      DO 10 J=1,N
      PLOT(J)=DASH
10    CONTINUE
      DO 11 J=IPLT,N,IPLT
      IF(J.LE.N) PLOT(J)=PLUS
11    CONTINUE
      WRITE(6,105) MASS,F,RELFRC,PLOT
      GOTO 8
19    WRITE(6,105) MASS,F,RELFRC
8     CONTINUE
C     FOR TTY CHANGE TO  50A1
105   FORMAT(I6,F11.7,F11.7,2X,100A1)
      WRITE(6,106) SUMM
106   FORMAT('0 TOTAL PROBABILITY =',F9.6,///)
      GOTO 50
51    STOP
      END
```

```
      SUBROUTINE DISEIS(AT,L,A,SUM,NIST)
      DIMENSION A(500),ATOM(15,85),ATAM(15,19),ATEM(15,19)
      DIMENSION ATIM(15,15),ATUM(15,18),ATYM(15,14)
          DATA ATAM/
     & ' H',1.,.999855,.000145,11*0.,
     & 'HE',3.,.00000137,.99999863,11*0.,
     & 'LI',6.,.0750,.9250,11*0.,
     & 'BE',9.,1.,12*0.,
     & ' B',10.,.1978,.8022,11*0.,
     & ' C',12.,.98888,.01112,11*0.,
     & ' N',14.,.99633,.00367,11*0.,
     & ' O',16.,.99759,.000374,.002039,10*0.,
     & ' F',19.,1.,12*0.,
     & 'NE',20.,.9092,.00257,.0882,10*0.,
     & 'NA',23.,1.,12*0.,
     & 'MG',24.,.7870,.1013,.1117,10*0.,
     & 'AL',27.,1.,12*0.,
     & 'SI',28.,.9221,.0470,.0309,10*0.,
     & ' P',31.,1.,12*0.,
     & ' S',32.,.95018,.00760,.04215,0.,.00014,8*0.,
     & 'CL',35.,.7553,.0,.2447,10*0.,
     & 'AR',36.,.00337,0.,.00063,0.,.99600,8*0.,
     & ' K',39.,.9310,.000118,.0688,10*0./
          DATA ATEM/
     & 'CA',40.,.9697,0.,.0064,.00145,.0206,0.,.00003,0.,.00185,4*0.,
     & 'SC',45.,1.,12*0.,
     & 'TI',46.,.0793,.0728,.7394,.0551,.0534,8*0.,
     & ' V',50.,.0024,.9976,11*0.,
     & 'CR',50.,.0431,0.,.8376,.0955,.0238,8*0.,
```

```
     & 'MN',55.,1.,12*0.,
     & 'FE',54.,.0582,0.,.9166,.0219,.0033,8*0.,
     & 'CO',59.,1.,12*0.,
     & 'NI',58.,.6788,0.,.2623,.0119,.0366,0.,.0108,6*0.,
     & 'CU',63.,.6909,0.,.3091,10*0.,
     & 'ZN',64.,.4889,0.,.2781,.0411,.1857,0.,.0062,6*0.,
     & 'GA',69.,.604,0.,.396,10*0.,
     & 'GE',70.,.2052,0.,.2743,.0776,.3654,0.,.0776,6*0.,
     & 'AS',75.,1.,12*0.,
     & 'SE',74.,.0087,0.,.0902,.0758,.2352,0.,.4982,0.,.0919,4*0.,
     & 'BR',79.,.50537,0.,.49463,10*0.,
     & 'KR',78.,.0035,0.,.0227,0.,.1156,.1155,.5690,0.,.1737,4*0.,
     & 'RB',85.,.7215,0.,.2785,10*0.,
     & 'SR',84.,.0056,0.,.0986,.0702,.8256,8*0./
        DATA ATIM/
     & ' Y',89.,1.,12*0.,
     & 'ZR',90.,.5146,.1123,.1711,0.,.1740,0.,.0280,6*0.,
     & 'NB',93.,1.,12*0.,
     & 'MO',92.,.1584,0.,.0904,.1572,.1653,.0946,.2378,0.,.0963,4*0.,
     & 'RU',96.,.0551,0.,.0187,.1272,.1262,.1707,.3163,0.,.1858,4*0.,
     & 'RH',103.,1.,12*0.,
     & 'PD',102.,.0096,0.,.1097,.2223,.2733,0.,.2671,0.,.1191,4*0.,
     & 'AG',107.,.51817,0.,.48183,10*0.,
     & 'CD',106.,.0122,0.,.0088,0.,.1239,.1275,.2407,.1226,.2886,0.,
     &     .0758,0.,0.,
     & 'IN',113.,.0428,0.,.9572,10*0.,
     & 'SN',112.,.0096,0.,.0066,.0035,.1430,.0761,.2403,.0858,.3285,0.,
     &     .0472,0.,.0594,
     & 'SB',121.,.5725,0.,.4275,10*0.,
     & 'TE',120.,.00089,0.,.0246,.0087,.0461,.0699,.1871,0.,.3179,0.,
     &     .3448,0.,0.,
     & ' I',127.,1.,12*0.,
     & 'XE',124.,.00096,0.,.00090,0.,.01919,.2644,.0408,.2118,.2689,
     &     0.,.1044,0.,.0887/
        DATA ATUM/
     & 'CS',133.,1.,12*0.,
     & 'BA',130.,.00101,0.,.00097,0.,.0242,.0659,.0781,.1132,.7166,4*0.,
     & 'LA',138.,.00089,.99911,11*0.,
     & 'CE',136.,.00193,0.,.00250,0.,.8848,0.,.1107,6*0.,
     & 'PR',141.,1.,12*0.,
     & 'ND',142.,.2711,.1217,.2385,.0830,.1722,0.,.0573,0.,.0562,4*0.,
     & 'SM',144.,.0309,0.,0.,.1497,.1124,.1383,.0744,0.,.2672,0.,
     &     .2271,0.,0.,
     & 'EU',151.,.4782,0.,.5218,10*0.,
     & 'GD',152.,.0020,0.,.0215,.1473,.2047,.1568,.2487,0.,.2190,4*0.,
     & 'TB',159.,1.,12*0.,
     & 'DY',156.,.00052,0.,.00090,0.,.0229,.1888,.2553,.2497,.2818,4*0.,
     & 'HO',165.,1.,12*0.,
     & 'ER',162.,.00136,0.,.0156,0.,.3341,.2294,.2707,0.,.1488,4*0.,
     & 'TM',169.,1.,12*0.,
     & 'YB',168.,.00135,0.,.0303,.1431,.2182,.1613,.3184,0.,.1273,4*0.,
     & 'LU',175.,.9741,.0259,11*0.,
     & 'HF',174.,.0018,0.,.0520,.1850,.2714,.1375,.3524,6*0.,
     & 'TA',180.,.00012,.99988,11*0./
        DATA ATYM/
     & ' W',180.,.0014,0.,.2641,.1440,.3064,0.,.2841,6*0.,
     & 'RE',185.,.3707,0.,.6293,10*0.,
```

```
     & 'OS',184.,.0002,0.,.0159,.0164,.133,.161,.264,0.,.410,4*0.,
     & 'IR',191.,.373,0.,.627,10*0.,
     & 'PT',190.,.00013,0.,.0078,0.,.329,.338,.253,0.,.0721,4*0.,
     & 'AU',197.,1.,12*0.,
     & 'HG',196.,.00146,0.,.1032,.1684,.2313,.1322,.2980,0.,.0685,4*0.,
     & 'TL',203.,.2950,0.,.7050,10*0.,
     & 'PB',204.,.0148,0.,.236,.226,.523,8*0.,
     & 'BI',209.,1.,12*0.,
     & 'TH',232.,1.,12*0.,
     & ' U',234.,.000057,.0072,0.,0.,.9927,8*0.,
     &      30*0./
      EQUIVALENCE(ATOM(1),ATAM(1)),(ATOM(286),ATEM(1)),(ATOM(571),
     & ATIM(1)),(ATOM(796),ATUM(1)),(ATOM(1066),ATYM(1))
      SUM=0.
      ATM=AT
      DO 1 I=1,85
      J=I
      IF(ATM.EQ.ATOM(1,I)) GOTO 2
1     CONTINUE
2     L=IFIX(ATOM(2,J))
      DO 3 I=1,13
      A(I)=ATOM(I+2,J)
      IF(A(I).LE.0.) GOTO 3
      SUM=SUM+A(I)
      NIST=I
3     CONTINUE
      RETURN
      END
```

APPENDIX B

LISTING OF COMPUTER PROGRAM FOR THE ASSIGNMENT OF MOLECULAR FORMULAS

```
      INTEGER ATOM(140),AMASS(9),ATM(9),L(9),J(9)
      DATA ATOM/' H',1,'LI',7,'BE',9,' B',11,' C',12,' N',14,'ME',15,
     & ' O',16,'OH',17,'WA',18,' F',19,'NE',20,'NA',23,'MG',24,'AL',27,
     & 'SI',28,' P',31,' S',32,'CL',35,'AR',40,' K',39,'CA',40,'SC',45,
     & 'TI',48,' V',51,'CR',52,'MN',55,'FE',56,'CO',59,'NI',58,'CU',63,
     & 'GA',69,'AS',75,'RB',72,'SR',88,' Y',89,'NB',93,'RH',103,
     & 'IN',96,' I',100,'CS',133,'BA',138,'LA',139,'CE',140,'PR',141,
     & 'TB',159,'HO',165,'TM',169,'LU',175,'TA',181,'RE',187,'IR',193,
     & 'AU',197,'TL',205,'BI',209,'TH',232,' U',238,
     & 24*0,
     & '  ',0/
      DATA YES/'Y'/
C     FOR TIME SHARING SYSTEMS REMOVE 'C' FROM I/O AND IF STATEMENTS
C     WRITE(6,200)
200   FORMAT('0ENTER ATOMS AS 9A2')
501   READ(5,100,END=500) ATM
100   FORMAT(9A2)
C     WRITE(6,201)
201   FORMAT('0ENTER M/E AS I4')
      READ(5,101) MOLMAS
101   FORMAT(I4)
      DO 1 I=1,9
      DO 2 K=1,99,2
      IF(ATM(I).NE.ATOM(K)) GOTO 2
      AMASS(I)=ATOM(K+1)
      GOTO 1
2     CONTINUE
1     CONTINUE
102   FORMAT('0MASS ',9A3)
      DO 5 I=1,9
      NB=I
      IF(ATM(I).EQ.ATOM(99)) GOTO 6
5     CONTINUE
      NB=NB+1
6     CONTINUE
17    NC=NB-1
      NCMB=1
      DO 16 II=1,NC
      L(II)=MOLMAS/AMASS(II)
      NCMB=(L(II)+1)*NCMB
16    CONTINUE
      WRITE(6,202) NCMB,(L(I),I=1,NC)
202   FORMAT('  THERE ARE',I10,' COMBINATIONS',/
     & '  MAX NO. OF EACH ATOM IS',9I3)
C     WRITE(6,109)
109   FORMAT('  DO YOU WISH TO RESET MAXIMUMS ')
C     READ(5,203) HUH
```

```
203   FORMAT(A1)
C     IF(HUH.NE.YES) GOTO 24
C     WRITE(6,204)
204   FORMAT('ENTER NO. ATOMS AS 9I2')
      READ(5,205)(L(I),I=1,NC)
205   FORMAT(9I2)
24    IMASS=0
      L1=L(1)+1
      L2=L(2)+1
      L3=L(3)+1
      L4=L(4)+1
      L5=L(5)+1
      L6=L(6)+1
      L7=L(7)+1
      L8=L(8)+1
      L9=L(9)+1
      WRITE(6,102)(ATM(I),I=1,NC)
      DO 30 I1=1,L1
      J(1)=I1-1
      M1=J(1)*AMASS(1)
      DO 30 I2=1,L2
      J(2)=I2-1
      M2=J(2)*AMASS(2)+M1
      DO 30 I3=1,L3
      J(3)=I3-1
      M3=J(3)*AMASS(3)+M2
      DO 30 I4=1,L4
      J(4)=I4-1
      M4=J(4)*AMASS(4)+M3
      DO 31 I5=1,L5
      J(5)=I5-1
      M5=J(5)*AMASS(5)+M4
      IF(M5.GT.MOLMAS) GOTO 30
      DO 32 I6=1,L6
      J(6)=I6-1
      M6=J(6)*AMASS(6)+M5
      IF(M6.GT.MOLMAS) GOTO 31
      DO 33 I7=1,L7
      J(7)=I7-1
      M7=J(7)*AMASS(7)+M6
      IF(M7.GT.MOLMAS) GOTO 32
      DO 34 I8=1,L8
      J(8)=I8-1
      M8=J(8)*AMASS(8)+M7
      IF(M8.GT.MOLMAS) GOTO 33
      DO 35 I9=1,L9
      J(9)=I9-1
      MSS=J(9)*AMASS(9)+M8
      IF(MOLMAS-MSS) 34,21,35
21    WRITE(6,108) MSS,(J(I),I=1,NC)
108   FORMAT(I5,9I3)
35    CONTINUE
34    CONTINUE
33    CONTINUE
32    CONTINUE
31    CONTINUE
30    CONTINUE
```

```
C       PRINT OUT OF MAX. NO. OF EACH ATOM (LEAVE OUT OF T/S VERSION)
        WRITE(6,104) (L(I),I=1,NC)
104     FORMAT(/5X,9I3,//)
        GOTO 501
500     STOP
        END
```

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```
run dismis
ENTER MOLECULE IN 10(A2,I2) FORMAT; RIGHT JUSTIFY
mo 3 o 9


 ISOTOPIC DISTRIBUTION FOR    MO 3 O 9

 ELEMENTAL DISTRIBUTIONS
  MO    92          93          94          95          96          97          98
      0.158400    0.000000    0.099400    0.157200    0.165300    0.094600    0.237800
       99         100
      0.000000    0.096300
   O   16          17          18
      0.997590    0.000374    0.002039

 MOLECULAR DISTRIBUTION
  M/E    ABSOLUTE    RELATIVE          1         2         3         4         5         6         7         8         9         10
  420  0.0038889  0.0371995  ----
  421  0.0000131  0.0001255
  422  0.0007299  0.0043744  ------
  423  0.0116012  0.1109701  ----------+-
  424  0.0161372  0.1543596  ----------+-----
  425  0.0204509  0.1956210  ----------+----------+
  426  0.0439892  0.4207762  ----------+----------+----------+----------+--
  427  0.0364112  0.3482888  ----------+----------+----------+-----
  428  0.0650705  0.6224263  ----------+----------+----------+----------+----------+----------+--
  429  0.0700511  0.6700698  ----------+----------+----------+----------+----------+----------+----------+-------
  430  0.0830748  0.7946470  ----------+----------+----------+----------+----------+----------+----------+----------+----------
  431  0.0841074  0.8045085  ----------+----------+----------+----------+----------+----------+----------+----------+----------+-
  432  0.1045430  1.0000000  ----------+----------+----------+----------+----------+----------+----------+----------+----------+----------+----------+----------+----------+
  433  0.0783243  0.7492059  ----------+----------+----------+----------+----------+----------+----------+----------+-----
  434  0.0980816  0.9381934  ----------+----------+----------+----------+----------+----------+----------+----------+----------+----------+----
  435  0.0700306  0.6698731  ----------+----------+----------+----------+----------+----------+----------+-------
  436  0.0683002  0.6533218  ----------+----------+----------+----------+----------+----------+-----
  437  0.0471772  0.4512710  ----------+----------+----------+----------+-----
  438  0.0417658  0.3995078  ----------+----------+----------+----------+
  439  0.0179891  0.1720758  ----------+-------
  440  0.0212988  0.2037324  ----------+----------+
  441  0.0029664  0.0283749  ---
  442  0.0068664  0.0656801  -------
  443  0.0000756  0.0006980
  444  0.0009962  0.0095295  -
  445  0.0000037  0.0000355
  446  0.0000171  0.0001633
  447  0.0000000  0.0000002
  448  0.0000001  0.0000012

 TOTAL PROBABILITY = 1.000017
```

(a) Molybdenum trioxide trimer.

Figure 1. - Isotopic distributions. Output taken from time-sharing version of program DISMIS.

```
run dismis
ENTER MOLECULE IN 10(A2,I2) FORMAT; RIGHT JUSTIFY
 c 4 h 4br 2cl 1 f 3


 ISOTOPIC DISTRIBUTION FOR      C 4 H 4BR 2CL 1 F 3

 ELEMENTAL DISTRIBUTIONS
   C   12          13
      0.988880    0.011120
   H    1           2
      0.999855    0.000145
  BR   79          80          81
      0.505370    0.000000    0.494630
  CL   35          36          37
      0.755300    0.000000    0.244700
   F   19
      1.000000

 MOLECULAR DISTRIBUTION
  M/E    ABSOLUTE    RELATIVE          1         2         3         4         5         6         7         8         9         10
  302   0.1843574   0.4381624  ---------+---------+---------+---------+----
  303   0.0083994   0.0199628  --
  304   0.4207512   1.0000000  ---------+---------+---------+---------+---------+---------+---------+---------+---------+---------+
  305   0.0191041   0.0455473  -----
  306   0.2938514   0.6983971  ---------+---------+---------+---------+---------+---------+---------+
  307   0.0133755   0.0317895  ---
  308   0.0574403   0.1365327  ---------+----
  309   0.0026088   0.0061998  -
  310   0.0000449   0.0001067
  311   0.0000004   0.0000008

 TOTAL PROBABILITY = 0.999999
```

(b) Dibromochlorotrifluorobutane.

Figure 1. - Concluded

```
run findme

ENTER ATOMS AS 9A2
 kclcr o

ENTER M/E AS I4
 294
THERE ARE       8208 COMBINATIONS
 MAX NO. OF EACH ATOM IS  7  8  5 18
 DO YOU WISH TO RESET MAXIMUMS?
no

MASS  K CL CR  O
 294  0  2  0 14
 294  0  2  4  1
 294  0  6  1  2
 294  1  1  3  4
 294  1  5  0  5
 294  2  0  2  7
 294  4  2  1  1
 294  5  1  0  4
```

(a) Potassium, chlorine, chromium, and oxygen for mass of 294 atomic mass units.

```
run findme

ENTER ATOMS AS 9A2
cr onaclohalsifenl

ENTER M/E AS I4
 118
THERE ARE     907200 COMBINATIONS
 MAX NO. OF EACH ATOM IS  2  7  5  3  6  4  4  2  2
 DO YOU WISH TO RESET MAXIMUMS?
yes

ENTER NO. ATOMS AS 9I2
 2 7 4 3 4 2 2 1 1

MASS CR  O NA CL OH AL SI FE NI
 118  0  0  0  0  2  0  1  1  0
 118  0  0  0  1  0  1  0  1  0
 118  0  0  0  1  0  1  2  0  0
 118  0  0  1  0  4  1  0  0  0
 118  0  0  2  0  1  1  1  0  0
 118  0  1  0  0  1  1  0  0  1
 118  0  1  1  0  3  0  1  0  0
 118  0  1  1  1  1  1  0  0  0
 118  0  1  2  0  0  0  0  1  0
 118  0  1  2  0  0  0  2  0  0
 118  0  2  0  0  0  0  1  0  1
 118  0  2  0  1  3  0  0  0  0
 118  0  2  1  1  0  0  1  0  0
 118  0  2  3  0  1  0  0  0  0
 118  0  3  0  2  0  0  0  0  0
 118  0  4  0  0  0  2  0  0  0
 118  1  1  1  0  0  1  0  0  0
 118  1  2  0  0  2  0  0  0  0
```

(b) Chromium, oxygen, sodium, chlorine, hydroxyl, aluminum, silicon, iron, and nickel for mass of 118 atomic mass units.

Figure 2. - Combinations of elements or radicals. Output taken from time-sharing version of program FINDME.

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