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Calculation of Any M$^+$ Value in Mass Spectrometry

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Abstract This paper discusses our "Dry Lab" experiment where students are shown the procedure for calculating the nominal and precise M$^+$ values of a compound. However, our main focus deals with the detailed step-by-step process for calculating the precise M^{+1} and M^{+2} values of a compound, as well as any of its higher order M$^+$ values, when its molecular formula is known.

Keywords: *calculation of M$^+$, calculation of M^{+1}, calculation of M^{+2}, organic chemistry, mass spectroscopy, instrumental analysis*

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1. Introduction

One of the topics taught in all organic chemistry courses is the identification of organic compounds. There are a number of wet chemistry methods as well as a number of instrumental methods for classifying and identifying organic compounds. Some very powerful instrumental methods involve the spectral data, and its interpretation, obtained from NMR, IR, UV, and mass spectrometry. Of the instrumental methods just mentioned, this paper will concentrate on mass spectroscopy. Mass spectral data not only provides the masses of the various fragments of molecules that are produced when molecules in the vapor phase are bombarded with a high-energy electron beam, but can furnish the mass of the molecular ion, M$^+$. A mass spectrum can also display one or more higher order M$^+$ peaks, for example, M^{+1} and M^{+2}, which taken together with the M$^+$ peak can be of value when identifying an unknown compound. In addition to a brief discussion regarding the calculation of a compound's M$^+$ value, a detailed step-by-step calculation of the higher order M$^+$ peaks, M^{+1} and M^{+2}, which arise as a consequence of the various isotopes of the elements that are in the compound being studied, are the main focus of this paper. We have included our computer program to aid instructors in preparing keys for the students which shows in detail all of the steps involved in these calculations.

2. Information Needed for Calculations

The information needed to make these calculations for this "Dry Lab" experiment are the molecular formula of the compound, some isotopic data of the elements in the compound, and the equations needed to calculate the value of M$^+$, M^{+1}, and M^{+2}. The isotopic data needed are the nominal and precise atomic masses of each of the major isotopes of each element in the compound, the percentage of each isotope of each element in the compound, and the number of significant figures in each of these percentages. The isotopic data used in this paper is listed in Table 1.

Table 1. Isotopic Data

Elements and Nominal Masses Given in Da[a]	Precise Masses of Isotopes to Six Decimal Places Given in Da[a] [1-3]	Isotope Percentages [1,4]	Significant Figures in Minor Isotope Percentages
H-1	1.007825	99.9885	
H-2		0.0115	3
C-12	12 (Exact)	98.93	
C-13		1.07	3
O-16	15.994915	99.757	
O-17		0.038	2
O-18		0.205	3
S-32	31.972071	94.99	
S-33		0.75	2
S-34		4.25	3
S-36		0.01	1
Br-79	78.918338	50.69	
Br-81		49.31	4

[a]1 Da = 1 u ("Da" is the symbol for daltons; "u" is the symbol for the unified atomic mass unit).

2.1. Calculation of the Nominal and Precise M$^+$ Values of $C_{27}H_{28}O_5SBr_2$-Bromothymol Blue

There are two M$^+$ quantities that are calculated below: the nominal and precise M$^+$ values. As can be seen in

Table 2, these calculations are straight forward requiring one to simply multiply the number of atoms of each element in the compound by its nominal mass found in Table 1 and then add each of these elements contribution to obtain the nominal M^+ value. The precise M^+ value, to six decimal places, is calculated in a like manner as shown in Table 3.

Table 2. Calculation of the Nominal Value of M^+

Isotope	Number of Atoms		Nominal Mass of Isotopes in Da		Contribution to M^+
H-1	28	x	1	=	28
C-12	27	x	12	=	324
O-16	5	x	16	=	80
S-32	1	x	32	=	32
Br-79	2	x	79	=	158
			Nominal M^+ Value =		622

Table 3. Calculation of the Precise Value of M^+

Isotope	Number of Atoms		Precise Mass of Isotopes in Da to Six Decimal Places[1-3]		Contribution to M^+
H-1	28	x	1.007825	=	28.219100
C-12	27	x	12 (Exact)	=	324
O-16	5	x	15.994915	=	79.974575
S-32	1	x	31.972071	=	31.972071
Br-79	2	x	78.918338	=	157.836676
			Precise M^+ Value =		622.002422

2.2. Calculation of the M^{+1} Value for $C_{27}H_{28}O_5SBr_2$-Bromothymol Blue

There is only one case or one group of isotopes to consider when calculating the value of the M^{+1} peak of bromothymol blue, the elements in the compound that have an M^{+1} isotope. Thus, one could begin by listing all of these elements as shown in the first column of Table 4. Then calculate the contribution that each one of these isotopes contributes toward the total value of the M^{+1} peak, starting in this example with hydrogen, the first isotope listed in Table 4. The quantity that hydrogen would contribute to the M^{+1} peak is calculated by taking the ratio of the percentage of the H-2 isotope divided by the percentage of the H-1 isotope times the number of hydrogens atoms in the compound times 100% [5]. This calculation just described is shown in red in Table 4. The next line in Table 4 has the appropriate numerical data substituted into the formula with the results of the calculation given in the right hand column. This process is repeated for each of the remaining isotopes listed in column 1 of Table 4. Adding all of these contributions and rounding the answer, showing just the significant figures, gives the value of the M^{+1} peak as a percentage of the intensity of the molecular ion peak, M^+. The reason there are so many decimal places included in these calculations was to demonstrate to the students how little some of the sets of isotopes actually contribute to these final calculated values.

Table 4. Calculation of the Precise Value of M^{+1}

Number of Each Isotope Contributing to M^{+1}	Calculation of M^{+1}	Percentage Contribution To M^{+1}
1 H-1	$\left(\left(\frac{\%\ of\ H-2\ isotope}{\%\ of\ H-1\ isotope}\right) * \ total\ \#\ of\ hydrogen\ atoms\right) * 100\%$	
1 H-1	$\left(\left(\frac{0.0115}{99.9885}\right) * 28\right) * 100\%$	0.3220370343
1 C -13	$\left(\left(\frac{\%\ of\ C-13\ isotope}{\%\ of\ C-12\ isotope}\right) * \ total\ \#\ of\ carbon\ atoms\right) * 100\%$	
1 C -13	$\left(\left(\frac{1.07}{98.93}\right) * 27\right) * 100\%$	29.2024663904
1 O-17	$\left(\left(\frac{\%\ of\ O-17\ isotope}{\%\ of\ O-16\ isotope}\right) * \ total\ \#\ of\ oxygen\ atoms\right) * 100\%$	
1 O-17	$\left(\left(\frac{0.038}{99.757}\right) * 5\right) * 100\%$	0.1904628247
1 S-33	$\left(\left(\frac{\%\ of\ S-33\ isotope}{\%\ of\ S-32\ isotope}\right) * \ total\ \#\ of\ sulfur\ atoms\right) * 100\%$	
1 S-33	$\left(\left(\frac{0.75}{94.99}\right) * 1\right) * 100\%$	0.7895567955
	M^{+1} =	30.5045230448
	Rounded Significant Figures M^{+1} =	30.5

2.3. Calculation of the M^{+2} Value for $C_{27}H_{28}O_5SBr_2$ - Bromothymol Blue

There are three cases to consider when calculating the M^{+2} value for bromothymol blue: (1) two M^{+1} isotopes of the same element, (2) two M^{+1} isotopes of different elements, and (3) one M^{+2} isotope of one element. In order to calculate the M^{+2} value, one could start by listing all the sets of the isotopes that will produce an M^{+2} value in the first column of Table 5. Then begin the calculations with the first set of isotopes listed for case 1 in Table 5, two H-2 isotopes of hydrogen. If there were just two hydrogen atoms in the molecule, the quantity they would contribute to the M^{+2} peak would be calculated by taking the ratio of the percentage of the H-2 isotope divided by the percentage of the H-1 isotope. This factor is repeated a second time for the second H-2 isotope, thus this ratio appears twice, once for each H-2 isotope. Another way of expressing this mathematically would be to write this ratio once and then square it, and then multiply that result by 100% [5]. However, bromothymol blue doesn't have just two hydrogen atoms in its formula, it has 28, so this squared ratio just mentioned must be multiplied be the number of ways that the two H-2 isotopes can occur among the 28 hydrogen atoms in the molecule [6,7], which mathematically speaking is the combination of 28 objects selected two at a time. The formula for calculating the number of combinations possible for this case is as follows: [(the total number of hydrogen atoms in the molecule) factorial] divided by [(the number of H-2 isotopes in the molecule) factorial times (the number of H-1 isotopes in the molecule) factorial)] [6,7]. This calculation just described is shown in red in Table 5 below.

The number of combinations that two H-2 isotopes have when the molecule contains 28 hydrogens is calculated as described above: (28!)/[(2!)(26!)] [6,7]. Another way of expressing this quantity mathematically is (28)(27)(26!)/[((2!)(26!)], which reduces to (28)(27)/2. The next line in Table 5 has the appropriate numerical data substituted into this formula with the results of the calculation being given in the right hand column. This process is then repeated for the two remaining examples of case 1 in Table 5, 2 C-13 and 2 O-17.

The next calculation discussed involves an example from case 2 where there are two different M^{+1} isotopes, 1 H-2 and 1 C-13, contributing to the value of M^{+2} for bromothymol blue. This calculation is similar to the calculation made for the M^{+1} value. Here the ratio of the percentage of the H-2 isotope is divided by the percentage of the H-1 isotope times the number of hydrogen atoms in the compound times the ratio of the percentage C-13 isotope divided by the percentage of the C-12 isotope times the number of carbon atoms in the compound [5,6,7] times 100%. This calculation just described is shown in red in Table 5. The next line in Table 5 has the appropriate values substituted into the formula with the results of the calculation given in the right hand column. This process is then repeated for the five remaining examples of case 2 in Table 5, 1 H-2 and 1 O-17, 1 H-2 and 1 S-33, 1 C-13 and 1 O-17, 1 C-13 and 1 S-33, 1 O-17 and 1 S-33.

The next calculation discussed involves an example from case 3 where there is only one atom of one isotope, 1 O-18, required to generate its contribution to the M^{+2} value for bromothymol blue. This calculation is similar to the calculations made for the M^{+1} value. Here the ratio of the percentage of the O-18 isotope is divided by the percentage of the O-16 isotope times the number of oxygen atoms in the compound times 100% [5,6,7]. This calculation just described is shown in red in Table 5. The next line in Table 5 has the values substituted into the formula with the results of the calculation given in the right hand column. This process is then repeated for the two remaining examples of case 3 in Table 5, 1 S-34 and 1 Br-81. Adding each of these contributions and rounding the answer, showing just the significant figures, gives the value of the M^{+2} peak as a percentage of the intensity of the molecular ion peak, M^{+}.

Table 5. Calculation of the Precise Value of M^{+2}

Number of Each Isotope Contributing to M^{+2}	Calculation of M^{+2}	Percentage Contribution To M^{+2}
2 H-2	$\left(\left(\left(\frac{\%\text{ of H}-2\text{ isotope}}{\%\text{ of H}-1\text{ isotope}}\right)^{\text{total \# of H}-2\text{ isotopes}}\right) * \left(\frac{(\text{total \# of H atoms})!}{(\text{total \# of H}-2\text{ isotopes})! * (\text{total \# of H}-1\text{ isotopes})!}\right)\right) * 100\%$	
2 H-2	$\left(\left(\left(\frac{0.0115}{99.9885}\right)^2\right) * \left(\frac{28 * 27}{2}\right)\right) * 100\%$	0.0005000200
1 H-2 1 C-13	$\left(\left(\left(\frac{\%\ of\ H-2\ isotope}{\%\ of\ H-1\ isotope}\right) * (total\ \#\ of\ H\ atoms)\right) * \left(\left(\frac{\%\ of\ C-13\ isotope}{\%\ of\ C-12\ isotope}\right) * (total\ \#\ C\ atoms)\right)\right) * 100\%$	
1 H-2 1 C-13	$\left(\left(\left(\frac{0.0115}{99.9885}\right) * 28\right) * \left(\left(\frac{1.07}{98.93}\right) * 27\right)\right) * 100\%$	0.0940427567

Number of Each Isotope Contributing to M^{+2}	Calculation of M^{+2}	Percentage Contribution To M^{+2}
1 H-2 1 O-17	$\left(\left(\left(\frac{\%\ of\ H-2\ isotope}{\%\ of\ H-1\ isotope}\right)*(total\ \#\ of\ H\ atoms)\right)*\left(\left(\frac{\%\ of\ O-17\ isotope}{\%\ of\ O-16\ isotope}\right)*(total\ \#\ O\ atoms)\right)\right)*100\%$	
1 H-2 1 O-17	$\left(\left(\left(\frac{0.0115}{99.9885}\right)*28\right)*\left(\left(\frac{0.038}{99.757}\right)*5\right)\right)*100\%$	0.0006133608
1 H-2 1 S-33	$\left(\left(\left(\frac{\%\ of\ H-2\ isotope}{\%\ of\ H-1\ isotope}\right)*(total\ \#\ of\ H\ atoms)\right)*\left(\left(\frac{\%\ of\ S-33\ isotope}{\%\ of\ S-32\ isotope}\right)*(total\ \#\ S\ atoms)\right)\right)*100\%$	
1 H-2 1 S-33	$\left(\left(\left(\frac{0.0115}{99.9885}\right)*28\right)*\left(\left(\frac{0.75}{94.99}\right)*1\right)\right)*100\%$	0.0025426653
2 C-13	$\left(\left(\left(\frac{\%\ of\ C-13\ isotope}{\%\ of\ C-12\ isotope}\right)^{total\ \#\ of\ C-13\ isotopes}\right)*\left(\frac{(total\ \#\ of\ C\ atoms)!}{(total\ \#\ of\ C-13\ isotopes)!*(total\ \#\ of\ C-12\ isotopes)!}\right)\right)*100\%$	
2 C-13	$\left(\left(\left(\frac{1.07}{98.93}\right)^{2}\right)*\left(\frac{27*26}{2}\right)\right)*100\%$	4.1059972454
1 C-13 1 O-17	$\left(\left(\left(\frac{\%\ of\ C-13\ isotope}{\%\ of\ C-12\ isotope}\right)*(total\ \#\ of\ C\ atoms)\right)*\left(\left(\frac{\%\ of\ O-17\ isotope}{\%\ of\ O-16\ isotope}\right)*(total\ \#\ O\ atoms)\right)\right)*100\%$	
1 C-13 1 O-17	$\left(\left(\left(\frac{1.07}{98.93}\right)*27\right)*\left(\left(\frac{0.038}{99.757}\right)*5\right)\right)*100\%$	0.0556198424
1 C-13 1 S-33	$\left(\left(\left(\frac{\%\ of\ C-13\ isotope}{\%\ of\ C-12\ isotope}\right)*(total\ \#\ of\ C\ atoms)\right)*\left(\left(\frac{(\%\ of\ S-33\ isotope)}{\%\ of\ S-32\ isotope}\right)*(total\ \#\ S\ atoms)\right)\right)*100\%$	
1 C-13 1 S-33	$\left(\left(\left(\frac{1.07}{98.93}\right)*27\right)*\left(\left(\frac{0.75}{94.99}\right)*1\right)\right)*100\%$	0.2305700578
2 O-17	$\left(\left(\left(\frac{\%\ of\ O-17\ isotope}{\%\ of\ O-16\ isotope}\right)^{total\ \#\ of\ O-17\ isotopes}\right)*\left(\frac{(total\ \#\ of\ O\ atoms)!}{(total\ \#\ of\ O-17\ isotopes)!*(total\ \#\ of\ O-16\ isotopes)!}\right)\right)*100\%$	
2 O-17	$\left(\left(\left(\frac{0.038}{99.757}\right)^{2}\right)*\left(\frac{5*4}{2}\right)\right)*100\%$	0.0001451044
1 O-1 1 S-33	$\left(\left(\left(\frac{\%\text{ of O}-17\text{ isotope}}{\%\text{ of O}-16\text{ isotope}}\right)*(\text{total \# of O atoms})\right)*\left(\left(\frac{(\%\text{ of S}-33\text{ isotope})}{\%\text{ of S}-32\text{ isotope}}\right)*(\text{total \# S atoms})\right)\right)*100\%$	
1 O-1 1 S-33	$\left(\left(\left(\frac{0.038}{99.757}\right)*5\right)*\left(\left(\frac{0.75}{94.99}\right)*1\right)\right)*100\%$	0.0015038122
1 O-18	$\left(\left(\frac{\%\ of\ O-18\ isotope}{\%\ of\ O-16\ isotope}\right)*(total\ \#\ of\ O\ atoms)\right)*100\%$	

Number of Each Isotope Contributing to M^{+2}	Calculation of M^{+2}	Percentage Contribution To M^{+2}
1 O-18	$\left(\left(\frac{0.205}{99.757}\right) * 5\right) * 100\%$	1.0274968173
1 S-34	$\left(\left(\frac{\% \text{ of } S-34 \text{ isotope}}{\% \text{ of } S-32 \text{ isotope}}\right) * (\text{total } \# \text{ of } S \text{ atoms})\right) * 100\%$	
1 S-34	$\left(\left(\frac{4.25}{94.99}\right) * 1\right) * 100\%$	4.4741551742
1 Br-81	$\left(\left(\frac{\% \text{ of } Br-81 \text{ isotope}}{\% \text{ of } Br-79 \text{ isotope}}\right) * (\text{total } \# \text{ of } Br \text{ atoms})\right) * 100\%$	
1 Br-81	$\left(\left(\frac{49.31}{50.69}\right) * 2\right) * 100\%$	194.5551390807
	M^{+2} =	204.5483259371
	Rounded Significant Figures M^{+2} =	204.5

3. Student Assignment and Results

After a detailed discussion of this material with the lab students, they were told to calculate the nominal and precise M^+ values as well as the M^{+1} and M^{+2} values for all the sets of isotopes that produce these values for butane, 1-bromobutane, 1,2-dibromobutane, 1,2,3-tribromobutane, 1,2,3,4-tetrabromobutane, and bromothymol blue. These papers were graded and returned the students, along with the key for each of these problems. There were three problems on the midterm lab test covering these calculations worth a total of 16 points. The students were asked to calculate the precise M^+ value worth 1 point, M^{+1} value worth 4 points, and the M^{+2} value worth 11 points, for C_5H_9OBr. Table 6 lists the grade distribution and average grade for each of these problems in columns 2, 3, and 4 with column 5 listing the students grade distribution based on their total points earned on these three problems. The class average of 60 students was 83.9.

Table 6. Test Results

Grade Range / Last Line List Average Grade for That Item	% Grade Distribution of the Precise M^+ Calculations	% Grade Distribution of M^{+1} Calculations	% Grade Distribution of M^{+2} Calculations	% Grade Distribution Based On Total Points Earned by Each Student
90-100	68.3	78.3	56.6	56.7
80-89	0.0	0.0	16.7	11.7
70-79	0.0	6.7	0.0	11.7
60-69	0.0	0.0	11.7	6.6
50-59	0.0	8.3	10.0	5.0
40-49	0.0	0.0	0.0	5.0
30-39	0.0	0.0	1.7	0.0
20-29	0.0	0.0	0.0	0.0
10-19	0.0	0.0	0.0	0.0
0-9	31.7	6.7	3.3	3.3
Average	68.3	87.5	83.9	83.9

4. Formula for Calculating Any of the Higher Order M^+ Values

When calculating any of the higher order M^+ values of a compound, be it M^{+1}, M^{+2}, M^{+3}, M^{+4}, etcetera, one should first list all of the sets of isotopes that will produce the M^+ value being sought. If there is just one element present in a set of isotopes, one takes the ratio of this minor isotope percentage to its major isotope percentage and raises that result to the power of the number of the isotopes of that minor isotope in the compound. This quantity is then multiplied by the number of combinations possible for the minor isotope amongst the total number of atoms of that element in the compound [5]. The number of combinations possible is calculated by taking the factorial of the total number of atoms of that element in the compound and divide it by the (factorial of the number of atoms of the minor isotope times the factorial of its number of atoms of the major isotope) [6,7]. Then multiply this result by 100%. The mathematical formula just described is shown below.

$$\left(\left(\frac{\%\text{ of minor isotope}}{\%\text{ of major isotope}}\right)^{(\#\text{of atoms of minor isotope})}\right) \cdot \left(\frac{(\#\text{of atoms of element})!}{(\#\text{of atoms of minor isotope})! \cdot (\#\text{of atoms of major isotope})!}\right) \cdot 100\% \quad (1)$$

If there are two different elements in a set of isotopes, the formula above is applied to each of the elements as shown below multiplied by 100%. Thus, when there are two elements in a set of isotopes when calculating their contribution to a higher order M^+ value the formula used would be:

$$\left(\left(\frac{\%\text{ of minor isotope}}{\%\text{ of major isotope}}\right)^{(\#\text{of atoms of minor isotope})}\right) \cdot \left(\frac{(\#\text{of atoms of element})!}{(\#\text{of atoms of minor isotope})! \cdot (\#\text{of atoms of major isotope})!}\right) \cdot \left(\left(\frac{\%\text{ of minor isotope}}{\%\text{ of major isotope}}\right)^{(\#\text{of atoms of minor isotope})}\right) \cdot \left(\frac{(\#\text{of atoms of element})!}{(\#\text{of atoms of minor isotope})! \cdot (\#\text{of atoms of major isotope})!}\right) \cdot 100\% \quad (2)$$

Thus, in order to calculate the value of any of the higher order M^+ values, all one needs to do is to apply formula 1 to each element that appears in a set of isotopes and then multiply that result by 100% [5]. This process is then repeated for all of the sets of isotopes that will produce the higher order M^+ value being calculated. The value of the desired higher order M^+ value is obtained when the sum of each of these calculations is rounded showing just the significant figures.

5. Calculating the M^+ Values Using Our Computer Program

All that the program requires of the user is to enter the formula and its name or identifier. That is all there is to it. All of the step-by-step calculations will be displayed on the screen as well as recorded in a disk file named from the formula and name or identifier entered into the program as mentioned above. All of this is explained in detail in the supporting information that will be provided along with the program, upon request. A typical run of the program is shown below for bromothymol blue.

Table 7. Sample Program Run for Bromothymol Blue

```
The print in red below indicates what is typed by the user.


calc-m+   (press the "enter" key)


                      WELCOME TO THE MASS SPECTROMETRY PROGRAM
                      ========================================


The  following  information  appearing  on  the  screen is stored on disk and may be
viewed anytime by opening the  file  titled  "calc-m+-program-information.txt"  with
WORD using the Courier New font with a font Size of 9 and margins of 1 inch.


This program accepts formulas containing ten elements:  carbon,  hydrogen, nitrogen,
oxygen, sulfur, phosphorus, fluorine, chlorine, bromine, and iodine.


The value of the M+ peak is calculated for formulas containing the  elements  listed
above.


The  intensity of the  M+1  and  M+2  peaks  are calculated as a  percentage  of the
intensity of the M+ peak for formulas containing the elements listed above.
```

```
All of the data needed for these calculations has been compiled in the program. When
the program is run for the first time, in any given directory/folder, the program
writes a copy of all of this compiled data into a data file in that directory/
folder. It is the data therein that is used for all the calculations for all of the
future program runs made in that directory/folder. If this data does not match the
data you wish to use, this text data file, "calc-m+-isotopic-data.txt", may be
modified with Microsoft WORD without needing to modify the program in any way. Be
sure to save the file as a ".txt" file. If you modify this file and then at some
point in the future you wish to use the original data compiled in the program, all
you need to do is to delete this ".txt" data file and then run the program. This
will produce the original data file with all of the data compiled in the program.




Enter the formula of your compound
Using either upper or lower case and
then press the "enter" key.
(Example: c2h6o or C2H6O) ----------------> c27h28o5sbr2 (press the "enter" key)




If you wish, you can enter the name of
the compound or any other identifier
up to a maximum of 48 characters or,      ************************************************
you may just press the "enter" key ---> bromothymol blue (press the "enter" key)
```

```
              CALCULATIONS FOR C27H28O5SBr2 -- BROMOTHYMOL BLUE
              ====================================================



The isotopic data compiled in this program was obtained from
nist.gov/pml/atomic-weights-and-isotopic-compositions-relative-atomic-masses,
Updated: January 2015. To view, paste this reference into your browser, press
the "enter" key, scroll and select "All Elements", "Pre-formatted ASCII
Table", "Most common isotopes", and then click "Get Data".


The data used by the program may be modified by editing the data file "calc-
m+-isotopic-data.txt" as described in the file "calc-m+-program-
information.txt."


The formula for calculating the number of combinations that exist for "n"
atoms of an isotope out of a total of "y" atoms of that element came from
Joseph K. Blizstein and Jessica Hwang, "Introduction to Probability", CRC
Press, Taylor & Francis Group, 2015, 14.


The formulas for calculating all the M+ values came from J. H. Beynon, "Mass
Spectrometry and its Application to Organic Chemistry," Elsevier, Amsterdam,
1960, 296.


The results of these calculations are printed to the screen as well as to a
disk file located in your current directory/folder using your "formula plus
its name or identifier" as the file name.


The reason for printing so many decimal places was to show the students how
little some of the isotope combinations really contribute to the final
calculated values.


When viewing the computer output below, a single asterisks, "*", means to
multiply the numbers on either side of it. When an "**2" is seen it means to
square the preceding number. When an "**3" is seen it means to cube the
preceding number, etc.
```

```
CALCULATION OF THE NOMINAL VALUE OF M+
========================================
                     Nominal     Da or u
           # of     Da or u   Contribution
Isotope    Atoms     Value       to M+

 H-1        28   *     1     =     28
 C-12       27   *    12     =    324
 O-16        5   *    16     =     80
 S-32        1   *    32     =     32
 Br-79       2   *    79     =    158
                                 ------
       Nominal M+ Value      =    622

CALCULATION OF THE PRECISE VALUE OF M+
==============================================
                      Precise       Da or u
           # of       Da or u    Contribution
Isotope    Atoms       Value         to M+

 H-1        28  *   1.007825  =    28.219100
 C-12       27  *  12.000000  =   324.000000
 O-16        5  *  15.994915  =    79.974575
 S-32        1  *  31.972071  =    31.972071
 Br-79       2  *  78.918338  =   157.836676
                                -------------
            Precise M+ Value  =   622.002422

 NUMBER OF EACH ISOTOPE                                                                  PERCENTAGE
      CONTRIBUTING                                                                      CONTRIBUTION
         TO M+1                            CALCULATION OF M+1                               TO M+1
========================   ====================================================     ===================
1 H-2                       ((0.0115/99.9885)*28)*100%                                =      0.3220370343
1 C-13                      ((1.07/98.93)*27)*100%                                    =     29.2024663904
1 O-17                      ((0.038/99.757)*5)*100%                                   =      0.1904628247
1 S-33                      ((0.75/94.99)*1)*100%                                     =      0.7895567955
                                                                                            ---------------
                                                                                M+1   =     30.5045230448
                                                          Rounded Significant Figures M+1   =     30.5
```

```
 NUMBER OF EACH ISOTOPE                                                              PERCENTAGE
      CONTRIBUTING                                                                  CONTRIBUTION
         TO M+2                            CALCULATION OF M+2                           TO M+2
========================  ====================================================   ===================
2 H-2                     (((((0.0115/99.9885)**2)*28)*27)/2)*100%              =      0.0005000200
1 H-2    1 C-13           (((0.0115/99.9885)*28)*((1.07/98.93)*27))*100%        =      0.0940427567
1 H-2    1 O-17           (((0.0115/99.9885)*28)*((0.038/99.757)*5))*100%       =      0.0006133608
1 H-2    1 S-33           (((0.0115/99.9885)*28)*((0.75/94.99)*1))*100%         =      0.0025426653
2 C-13                    (((((1.07/98.93)**2)*27)*26)/2)*100%                  =      4.1059972454
1 C-13   1 O-17           (((1.07/98.93)*27)*((0.038/99.757)*5))*100%           =      0.0556198424
1 C-13   1 S-33           (((1.07/98.93)*27)*((0.75/94.99)*1))*100%             =      0.2305700578
2 O-17                    (((((0.038/99.757)**2)*5)*4)/2)*100%                  =      0.0001451044
1 O-17   1 S-33           (((0.038/99.757)*5)*((0.75/94.99)*1))*100%            =      0.0015038122
1 O-18                    ((0.205/99.757)*5)*100%                               =      1.0274968173
1 S-34                    ((4.25/94.99)*1)*100%                                 =      4.4741551742
1 Br-81                   ((49.31/50.69)*2)*100%                                =    194.5551390807
                                                                                    -----------------
                                                                         M+2    =    204.5483259371
                                                   Rounded Significant Figures M+2  =    204.5


type                         y   to do another calculation or
       <press the "enter" key   if you are finished
                        --->    (press the "enter" key)


All of the calculations from this program run
    are recorded in the following file: "C27H28O5SBr2  --  BROMOTHYMOL BLUE"
   To print this output file
      start "WORD" and then open the output file
      set the top and bottom margins to 0.7 inches (or as needed)
      set the right and left margins to 0.5 inches (or as needed)
      set the font to Courier New (a fixed width font is required
          so all of the numbers and decimals line up in the correct column)
      set the font size to 5.5 - 7 so the file prints on one page)
      and then click the print button
```

Statement of Competing Interests

The authors have no competing interest.

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