Calculation of Any M⁺ Value in Mass Spectrometry

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Received July 06, 2020; Revised August 08, 2020; Accepted August 17, 2020

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

Cite This Article: Andrew M. Kelley, Stephanie Garcia, David R. Khan, William G. Ambrose, Jason C. Yarbrough, James D. Woodyard, and James C. Espinosa, “Calculation of Any M⁺ Value in Mass Spectrometry.” World Journal of Chemical Education, vol. 8, no. 4 (2020): 141-149. doi: 10.12691/wjce-8-4-1.

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 Da¹ | Precise Masses of Isotopes to Six Decimal Places Given in Da[1-3] | Isotope Percentages [1,4] | Significant Figures in Minor Isotope Percentages |
|----------------------------------------|---------------------------------------------------------------|--------------------------|-----------------------------------------------|
| H-1                                    | 1.007825                                                      | 99.9885                  |                                               |
| H-2                                    | 0.0115                                                        |                          |                                               |
| C-12                                   | 12 (Exact)                                                   | 98.93                    |                                               |
| C-13                                   | 1.07                                                         |                          |                                               |
| O-16                                   | 15.994915                                                    | 99.757                   |                                               |
| O-17                                   | 0.038                                                        |                          |                                               |
| O-18                                   | 0.205                                                        |                          |                                               |
| S-32                                   | 31.972071                                                    | 94.99                    |                                               |
| S-33                                   | 0.75                                                         |                          |                                               |
| S-34                                   | 4.25                                                         |                          |                                               |
| S-36                                   | 0.01                                                         |                          |                                               |
| Br-79                                  | 78.918338                                                   | 50.69                    |                                               |
| Br-81                                  | 49.31                                                        |                          |                                               |

¹1 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 C₂₇H₂₈O₅SBr₂-
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 straightforward 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           | 1.007825                      | 28                |
| C-12    | 27 x           | 12.000000 (Exact)             | 324               |
| O-16    | 5 x            | 16.000000                     | 80                |
| S-32    | 1 x            | 32.000000                     | 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           | 12.000000 (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

### 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                                      | \( \left( \frac{\% \text{ of } H - 2 \text{ isotope}}{\% \text{ of } H - 1 \text{ isotope}} \right) \times \text{total # of hydrogen atoms} \times 100\% \)                                                                 | 0.3220370343                |
| 1 H-1                                      | \( \left( \frac{0.0115}{0.999885} \right) \times 28 \times 100\% \)                                                                                                                                               | 0.3220370343                |
| 1 C-13                                     | \( \left( \frac{\% \text{ of } C - 13 \text{ isotope}}{\% \text{ of } C - 12 \text{ isotope}} \right) \times \text{total # of carbon atoms} \times 100\% \)                                                          | 29.2024663904               |
| 1 C-13                                     | \( \left( \frac{1.07}{98.93} \right) \times 27 \times 100\% \)                                                                                                                                              | 29.2024663904               |
| 1 O-17                                     | \( \left( \frac{\% \text{ of } O - 17 \text{ isotope}}{\% \text{ of } O - 16 \text{ isotope}} \right) \times \text{total # of oxygen atoms} \times 100\% \)                                                  | 0.1904628247                |
| 1 O-17                                     | \( \left( \frac{0.38}{0.37} \right) \times 5 \times 100\% \)                                                                                                                                                  | 0.1904628247                |
| 1 S-33                                     | \( \left( \frac{\% \text{ of } S - 33 \text{ isotope}}{\% \text{ of } S - 32 \text{ isotope}} \right) \times \text{total # of sulfur atoms} \times 100\% \)                                                          | 0.789567955                 |
| 1 S-33                                     | \( \left( \frac{0.75}{94.99} \right) \times 1 \times 100\% \)                                                                                                                                              | 0.789567955                 |

\[ M'1 = \text{30.5} \]

Rounded Significant Figures \( M'1 = 30.5 \)
2.3. Calculation of the M$^{+2}$ Value for C$_{27}$H$_{28}$O$_{5}$SBr$_{2}$ - 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 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.

Another way of expressing this quantity mathematically is (28)(27)(26!)/[(2!)(26!)], which reduces to (28)(27)/2.

The number of hydrogen atoms in the compound times the ratio of the percentage C-13 isotope divided by the percentage C-12 isotope times 100% [5,6,7] 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 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 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 100% [5,6,7]. 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                                          | ( % of H – 2 isotope / % of H – 1 isotope ) = (total # of H – 2 isotopes)! / (total # of H – 2 isotopes)! * 100% | 0.0005000200 |
| 2 H-2                                          | ( % of H – 2 isotope / % of H – 1 isotope ) * (28 * 27 / 2) * 100% | 0.0940427567 |
| 1 H-2, 1 C-13                                 | ( % of H – 2 isotope / % of H – 1 isotope ) * (total # of H atoms) = (total # of H atoms)! / (total # of H – 2 isotopes)! * 100% | |
| 1 H-2, 1 C-13                                 | ( % of C – 13 isotope / % of C – 12 isotope ) * (total # C atoms) * 100% | |
| 1 H-2, 1 C-13                                 | ( % of H – 2 isotope / % of H – 1 isotope ) * (total # of H atoms) = (total # of H atoms)! / (total # of H – 2 isotopes)! * 100% | |
| 1 H-2, 1 C-13                                 | ( % of C – 13 isotope / % of C – 12 isotope ) * (total # C atoms) * 100% | |
| Number of Each Isotope Contributing to M² | Calculation of M²                    | Percentage Contribution To M² |
|----------------------------------------|--------------------------------------|-------------------------------|
| 1 H-2                                  | \(\left(\frac{\% \text{ of } H - 2 \text{ isotope}}{\% \text{ of } H - 1 \text{ isotope}}\right) \times \left(\frac{\% \text{ of } O - 17 \text{ isotope}}{\% \text{ of } O - 16 \text{ isotope}}\right) \times 100\%\) | 0.0006133608                  |
| 1 O-17                                 | \(\left(\frac{0.115}{0.99885} \times 28\right) \times \left(\frac{0.038}{0.99757} \times 5\right) \times 100\%\) | 0.0025426653                  |
| 1 H-2                                  | \(\left(\frac{\% \text{ of } H - 2 \text{ isotope}}{\% \text{ of } H - 1 \text{ isotope}}\right) \times \left(\frac{\% \text{ of } O - 17 \text{ isotope}}{\% \text{ of } O - 16 \text{ isotope}}\right) \times 100\%\) | 0.0006133608                  |
| 1 O-17                                 | \(\left(\frac{0.115}{0.99885} \times 28\right) \times \left(\frac{0.75}{0.9499} \times 1\right) \times 100\%\) | 0.001451044                   |
| 1 S-33                                 | \(\left(\frac{\% \text{ of } O - 17 \text{ isotope}}{\% \text{ of } O - 16 \text{ isotope}}\right) \times 100\%\) | 0.0015038122                  |
| 2 C-13                                 | \(\left(\frac{0.17}{0.9893} \times \frac{27 \times 26}{2}\right) \times 100\%\) | 4.1059972454                  |
| 2 C-13                                 | \(\left(\frac{\% \text{ of } C - 13 \text{ isotope}}{\% \text{ of } C - 12 \text{ isotope}}\right) \times \left(\frac{\% \text{ of } C \text{ - 13 isotopes}}{\% \text{ of } C \text{ - 13 isotopes}}\right) \times 100\%\) | 0.0556198424                  |
| 1 S-33                                 | \(\left(\frac{\% \text{ of } O - 17 \text{ isotope}}{\% \text{ of } O - 16 \text{ isotope}}\right) \times 100\%\) | 0.001451044                   |
| 2 O-17                                 | \(\left(\frac{\% \text{ of } O - 17 \text{ isotope}}{\% \text{ of } O - 16 \text{ isotope}}\right) \times \left(\frac{(\% \text{ of } O - 17 \text{ isotope}) !}{(\% \text{ of } O - 17 \text{ isotope}) ! \times (\% \text{ of } O - 16 \text{ isotope}) !}\right) \times 100\%\) | 0.001451044                   |
| 1 S-33                                 | \(\left(\frac{\% \text{ of } O - 17 \text{ isotope}}{\% \text{ of } O - 16 \text{ isotope}}\right) \times \left(\frac{(\% \text{ of } S - 33 \text{ isotope}) !}{(\% \text{ of } S - 33 \text{ isotope}) ! \times (\% \text{ of } S - 32 \text{ isotope}) !}\right) \times 100\%\) | 0.001451044                   |
| 1 S-33                                 | \(\left(\frac{\% \text{ of } O - 17 \text{ isotope}}{\% \text{ of } O - 16 \text{ isotope}}\right) \times \left(\frac{(\% \text{ of } S - 33 \text{ isotope}) !}{(\% \text{ of } S - 33 \text{ isotope}) ! \times (\% \text{ of } S - 32 \text{ isotope}) !}\right) \times 100\%\) | 0.001451044                   |
| 1 O-18                                 | \(\left(\frac{\% \text{ of } O - 18 \text{ isotope}}{\% \text{ of } O - 16 \text{ isotope}}\right) \times 100\%\) | 0.001451044                   |
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, 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$_2$H$_5$OBr. 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.

| Number of Each Isotope Contributing to M$^+$ | Calculation of M$^+$ | Percentage Contribution To M$^+$ |
|---------------------------------------------|-----------------------|----------------------------------|
| 1 O-18                                      | (0.205 \(\frac{99.737}{99.737}\)) \(\times 5\) \(\times 100\%\) | 1.0274968173                     |
| 1 S-34                                      | \(\frac{\% \text{ of } S - 34 \text{ isotope}}{\% \text{ of } S - 32 \text{ isotope}}\) \(\times (\text{total } \# \text{ of } S \text{ atoms})\) \(\times 100\%\) | 4.4741551742                     |
| 1 S-34                                      | (4.25 \(\frac{94.99}{99.99}\)) \(\times 1\) \(\times 100\%\) | 4.4741551742                     |
| 1 Br-81                                     | \(\frac{\% \text{ of } Br - 81 \text{ isotope}}{\% \text{ of } Br - 79 \text{ isotope}}\) \(\times (\text{total } \# \text{ of } Br \text{ atoms})\) \(\times 100\%\) | 194.5551390807                   |
| 1 Br-81                                     | (49.31 \(\frac{50.69}{100}\)) \(\times 2\) \(\times 100\%\) | 194.5551390807                   |

Rounded Significant Figures M$^+$ = 204.5

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.

\[
\left(\frac{\% \text{ of minor isotope}}{\% \text{ of major isotope}}\right)^{\text{(#of atoms of minor isotope)}} \times \left(\frac{\text{(#of atoms of element)!}}{\text{(#of atoms of minor isotope)!} \times \text{(#of atoms of major isotope)!}}\right) \times 100\% \tag{1}
\]

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:
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
===============================================

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.
(Examples: c2h6o or c2h6o) ~~~~~~~~~~ e27h20c5abr2 (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 E. Blaisdell 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 asterisk, "+", 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 Value of M+ | Contribution to M+ |
|---------------------|--------------------|
| Isotope | Atoms | Value | to M+ |
| H-1 | 20 | +1 | 20 |
| C-12 | 27 | +12 | 324 |
| O-16 | 8 | +16 | 80 |
| S-32 | 1 | +32 | 32 |
| Br-79 | 2 | +79 | 158 |
| Nominal M+ Value | 622 |

CALCULATION OF THE PRECISE VALUE OF M+

| Precise Value of M+ | Contribution to M+ |
|---------------------|--------------------|
| Isotope | Atoms | Value | to M+ |
| H-1 | 20 | 1 | 1.0070325 | 20.1219100 |
| C-12 | 27 | 12 | 12.0000000 | 924.0000000 |
| O-16 | 8 | 16 | 15.994915 | 79.9748575 |
| S-32 | 1 | 32 | 31.972071 | 31.972071 |
| Br-79 | 2 | 79 | 78.918338 | 157.836676 |
| Precise M+ Value | 622.002422 |

NUMBER OF EACH ISOTOPE CONTRIBUTING TO M+:

| Isotope | Percentage Contribution to M+ |
|---------|--------------------------------|
| H-2 | 0.3220370343 |
| O-13 | 29.2024663904 |
| S-32 | 0.1904628247 |
| Br-79 | 0.7895567556 |
| M-1 | 30.045330448 |

Rounded Significant Figures M-1 = 30.5

NUMBER OF EACH ISOTOPE CONTRIBUTING TO M+:

| Isotope | Calculation of M+ |
|---------|--------------------|
| H-2 | (((0.0115/99.9885)*28)*((1.07/99.95)*27)) / 100 |
| C-12 | (((0.0115/99.9885)*28)*((0.038/99.757)*5)) / 100 |
| O-16 | (((0.0115/99.9885)*28)*((0.75/94.98)*1)) / 100 |
| S-32 | ((1.07/99.93)*27) / 100 |
| Br-79 | (((0.038/99.757)*5)) / 100 |
| M-2 | (((0.038/99.757)*5)) / 100 |
| S-34 | ((4.25/94.99)*1) / 100 |
| Br-81 | (((45.31/50.69)*2)) / 100 |
| M+ | 204.549265971 |

Type "y" to do another calculation or "n" if you are finished

All of the calculations from this program run are recorded in the following file: "C2H8O6S8Br2 -- BRONOTHINOL BLUE"

To print this output file, set the top and bottom margins to 0.7 inches (or as needed), set the right and left margins to 0.8 inches (or as needed), set the font to Courier New (a fixed width font is required), set the printer to 100%, and print the file.
Statement of Competing Interests

The authors have no competing interest.

Acknowledgements

We thank the Department of Chemistry and Physics of West Texas A&M University for their financial support of this project.

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