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Relative Abundance Determination for more than Two Isotopes of an Element

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Eventhough the atomic weight (mass) of an element through mass spectra data is obtained by summing the products of the fractional or relative abundance of an isotope and the mass of that isotope [1] and eventhough the relative abundance for two isotopes can be obtained when the atomic mass and the mass of the isotopes are given as in the cases of boron [2] and silver [3], consideration should be given to determining the relative abundance for more than two isotopes.

In addition to $\Sigma f_n m_n$ = a.m. (translation of the above statement to a mathematical formula), $\Sigma f_n = 1$ (sum of all the relative abundances equals one) is an item of importance. These equations suffice for two isotopes in that there only are two equations in two unknowns and the solutions are obtained analytically [4].

The above summations also apply to more than two isotopes. However, there are two equations in n unknowns where n is the number of isotopes and this means an infinity of solutions [5] but in order for only one solution to be the case, there must be n equations in n unknowns. Nevertheless, two of the infinity of solutions should suffice and since this is an application to relative abundance determination, all the solutions must be positive numbers between zero and one.

In citing examples based on the above information, f_n will be replaced by RA_n. Hence $\Sigma RA_n m_n$ = a.m. and $\Sigma RA_n = 1$.

Example 1

Find two possible relative abundances for the isotopes of magnesium having masses of 23.98504, 24.98584 and 25.98259 given that the atomic mass of magnesium is 24.30955.

Here is an element with three isotopes. Hence the needed equations are $23.98504RA_1 + 24.98584RA_2 + 25.98259RA_3 = 24.30955$ and $1.00000RA_1 + 1.00000RA_2 + 1.00000RA_3 = 1.00000$. By executing the needed eliminations, RA_1 and RA_2 in terms of RA_3 are found to be $RA_1 = (0.67629 + 0.99675RA_3)/1.00080$ and RA_2 $(0.32451 - 1.99755RA_3)/1.00080$ respectively. Now a value less than 0.1630 will be substituted for RA_3 so that RA_1 and RA_2 will be positive and less than one. If $RA_3 = 0.1623$, then $RA_1 = 0.8374$ and $RA_2 = 0.0003$. The values of RA_1, RA_2 and RA_3 all add up to 1.0000. Now if $RA_3 = 0.1111$, RA_1 and RA_2 are 0.7864 and 0.1025 respectively. These results also add up to 1.0000.

Example 2

Find two possible relative abundances for the isotopes of neon having masses of 19.99244, 20.99395 and 21.99138 given that the atomic mass of neon is 20.17135.

This is another element with three isotopes and the needed equations are $19.99244RA_1 + 20.99395RA_2 + 21.99138RA_3 = 20.17135$ and $1.00000RA_1 + 1.00000RA_2 + 1.00000RA_3 = 1.00000$. Respective eliminations result in $RA_1 = (0.82260 + 0.99743RA_3)/1.00151$ and $RA_2 = (0.17891 - 1.99894RA_3)/1.00151$. Now a value less than 0.0910 will be assigned to RA_3 for RA_1 and RA_2 to be positive and less than one. If $RA_3 = 0.0880$, then $RA_1 = 0.9090$ and $RA_2 = 0.0030$. These values all add up to 1.0000. Now if $RA_3 = 0.0376$, $RA_1 = 0.8589$ and $RA_2 = 0.1035$. These values also add up to 1.0000.

Example 3

Obtain two possible relative abundances for the isotopes of chromium having masses of 49.9461, 51.9405, 52.9407 and 53.9389 given that the atomic mass of chromium is 51.9977.

Here now is an element with four isotopes and the needed equations are $49.9461RA_1 + 51.9405RA_2 + 52.9407RA_3 + 53.9389RA_4 = 51.9977$ and $1.0000RA_1 + 1.0000RA_2 + 1.0000RA_3 + 1.0000RA_4 = 1.0000$. Respective eliminations result in $RA_1 = (1.0002RA_3 + 1.9984RA_4 - 0.0572)/1.9944$ and $RA_2 = (2.0516 - 2.9946RA_3 - 3.9928RA_4)/1.9944$. If $RA_3 = 0.0975$ and $RA_4 = 0.0225$, $RA_1 = 0.0427$ and $RA_2 = 0.8373$. These values are summed up to 1.0000. Now if $RA_4 = RA_3 = 0.1000$, $RA_1 = 0.1216$ and $RA_2 = 0.6786$. These values also are summed up to 1.0000. In these and other cases RA_3 and RA_4 must be assigned positive values less than one so that RA_1 and RA_2 will be less than one and positive.

Final example

What are two possible relative abundances for the isotopes of iron having masses of 53.9396, 55.9349, 56.9354 and 57.9333 given that the atomic mass of iron is 55.8473.

This is another element with four isotopes and the needed equations are $53.9396RA_1 + 55.9349RA_2 + 56.9354RA_3 + 57.9333RA_4 = 55.8473$ and $1.0000RA_1 + 1.0000RA_2 + 1.0000RA_3 +$

$1.0000RA_4 = 1.0000$. Respective eliminations result in $RA_1 = (1.0005RA_3 + 1.9984RA_4 + 0.0876)/1.9953$ and $RA_2 = (1.9077 - 2.9958RA_3 - 3.9937RA_4)/1.9953$. If $RA_3 = 0.0204$ and $RA_4 = 0.0027$, $RA_1 = 0.0568$ and $RA_2 = 0.9202$. These values all add up to 1.0000. Now if $RA_4 = 4RA_3$ and $RA_3 = 0.0800$, $RA_4 = 0.3200$, $RA_1 = 0.4045$ and $RA_2 = 0.1955$. These values also add up to 1.0000. Even here RA_3 and RA_4 must be assigned positive values less than one so that RA_1 and RA_2 will be positive and less than one.

The above process applies to all elements with three and with four isotopes and it applies to all elements with more than four isotopes but more assignments are needed to solve the given system of equations.

References

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