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Letters

Understanding Isotopic Distributions in Mass Spectrometry

The article "Using Punnet Squares to Facilitate Students' Understanding of Isotopic Distributions in Mass Spectrometry" by Lawrence T. Sein, Jr. *(1)* is an interesting attempt to promote the understanding of the construction of isotopic distributions at the same time showing an interesting relationship between the isotope patterns and genetic traits. Here I want to bring to your attention an alternative simple graphical tool for obtaining complex isotopic distributions.

It is known that isotope patterns of molecules and ions form according to the binomial expansion *(2)*. The perennial Pascal's triangle is a graphical form of such an expansion and it is easy to see that the coefficients in the standard Pascal's triangle resemble the isotope patterns of bromine. Although the use of Pascal's triangle is widely advocated in textbook explanations of multiplets in ^{1}H NMR spectra, considerably less attention is paid to the fact that isotopic distributions of molecules can be explained in a similar fashion. As a slight modification of the standard Pascal's triangle, isotopic distributions can be rendered in the form of cellular automata, which generate complex isotopic patterns in an educationally friendly manner *(3)*.

As an example, the isotope pattern of $PbCl_2$ can be considered. Lead has three isotopes in a ratio of ~1:1:2 (^{206}Pb, ^{207}Pb, and ^{208}Pb) and chlorine has two isotopes in a ratio of ~3:1 (^{35}Cl and ^{37}Cl). The rather complex isotopic distribution of $PbCl_2$ can be easily obtained as shown in Figure 1. In this process, the isotopic distribution of $PbCl_2$ is obtained in two consecutive steps: first, the isotopic distribution of Cl_2 is obtained and then the isotopic distribution of Pb is added leading to the $PbCl_2$. Such construction of complex isotope patterns captures the very essence of the problem—complex isotope patterns can be generated using very simple rules. As can be seen from the above example, no calculators are needed to obtain the isotopic distribution of $PbCl_2$.

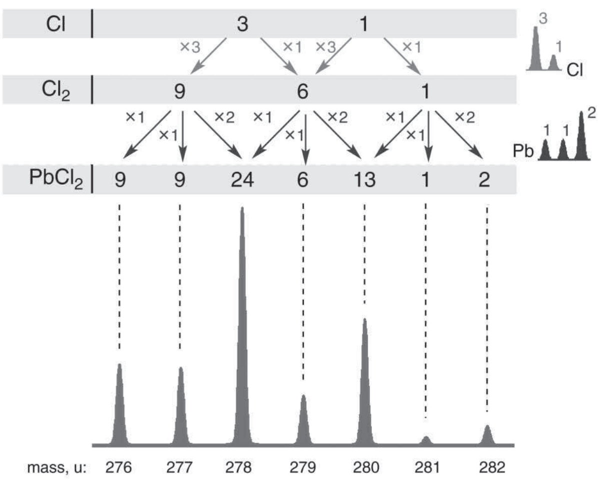

Figure 1. Complex isotopic distribution of $PbCl_2$.

Literature Cited

1. Sein, Lawrence T., Jr. *J. Chem. Educ.* **2006,** *83*, 228–232.
2. Margrave, J. L.; Polansky, R. B. *J. Chem. Educ.* **1962,** *39*, 335–337.
3. Meija, J. *Anal. Bioanal. Chem.* **2006,** *385*, 486–499.

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