Reinforcing Isotope and Atomic-Weight Concepts in General Chemistry Using Internet-Based Mass-Spectral Data

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Abstract: This paper describes how isotope and atomic-weight concepts are enhanced for students using mass-spectral data from interactive Internet sites. The class considers mass spectra for compounds containing only monoisotopic elements and later for polyisotopic elements. Students calculate molecular weights based on data they acquire from mass spectra on the Internet.

Introduction

Because biomedical, forensic, and environmental laboratories routinely use GC/MS (gas chromatography with mass spectrometry detection), students benefit from early exposure to this instrumentation, preferably at the general chemistry level. Student interest often increases when this introduction incorporates hands-on experience.

General chemistry students benefit from the study of mass spectrometry as it pertains to isotopes and atomic weights. Most general chemistry students easily find the atomic weight of an element on a periodic table, but some struggle with its meaning. When asked the mass of a chlorine atom, many answer 35.45 atomic mass units. Several papers [1] describe methods in which students use a mass spectrometer to gain a better understanding of isotopes, isotopic weights, and their relation to atomic weights. Many institutions, however, do not own the necessary equipment or serve too many students for individual use of the instrument. In this circumstance, an instructor might choose to use an overhead transparency of a mass spectrum for the discussion. While the use of transparencies provides the essential information for discussion, it can allow students to be passive learners. Alternatively, the Internet provides individual students with access to mass-spectral data from a broad range of chemical compounds and encourages them to be active learners. In a laboratory or classroom equipped with computers connected to the Internet, several students can access the data simultaneously or view spectra from different compounds. Use of the Internet to obtain spectra maintains the advantages of interactive discovery of data without the requirement of access to a spectrometer or exposure to unreasonably hazardous substances.

The Internet Sites

As with much of the Internet, many educational sites (perhaps some described here) often change, move, or disappear at the end of the quarter or semester. While not always possible, we attempt to mainly use sites that appear to be more or less permanent.

Several mass spectrometry tutorials are currently available via the Internet [2]. Though perhaps not designed specifically for general chemistry students, these sites offer good, general descriptions of mass spectrometry. Alternatively, general chemistry textbooks often present adequate descriptions of mass spectrometry [3].

The National Institute of Standards and Technology's Chemistry Webbook [4] contains real mass-spectral data that students can view interactively. From this page, students search for compounds by formula, name, or CAS registry number. The site displays available spectra in the normal bar-graph mode. Using the mouse and various option keys, students can explore the spectrum in detail and expand regions of interest. By moving the cursor over the top of a peak, students find the relative abundance of each ion. The page also provides printer-friendly spectra.

The Sheffield Chemputer [5] presents synthesized mass spectra based on isotopic weights and abundances. Due to the synthetic nature of the data, students can view "spectra" for virtually any compound. This also means, however, that the spectra lack fragmentation patterns, leaving only the molecular ion peaks. The Sheffield Chemputer presents data graphically as a traditional plot of abundance versus mass-to-charge ratio. Viewers also see relative-abundance data for all species presented numerically.

The Approach

During a lecture session, as part of either the laboratory or the lecture course, the instructor describes the basic theory and design of a mass spectrometer. Using the NIST WebBook and a video projector (alternatively, the students view the data on individual computers), the instructor presents the mass spectrum of a compound containing only monoisotopic elements (such as PF_3 or H_2O). (For the purposes of this discussion, we consider elements with 99.5% or more abundance of the primary isotope to be monoisotopic.) After identifying the molecular-ion peak, the students calculate the molecular weight based on the formula and compare it to the mass-to-charge ratio for the molecular-ion peak. The presence of additional peaks in the mass spectrum allows for a brief discussion of fragmentation patterns observed in mass spectra. This particular example (PF_3) shows peaks corresponding to the loss of one, two, and three fluorine radicals from the molecular ion.

The class then views a spectrum for a compound containing a polyisotopic element. Chlorine dioxide (ClO_2) is a good example because the chlorine isotope pattern (75.8% ^{35}Cl and 24.2% ^{37}Cl) is easily observed. Because oxygen is 99.8% ^{16}O,

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the other oxygen isotopes do not affect the observed mass spectrum or calculations. The students then explain the presence of the two peaks in the molecular-ion region and compare the calculated molecular weight of the compound to the mass-to-charge ratio for each molecular-ion peak. This illustration provides a springboard to the discussion of the relationship between molecular weight and isotopic abundance. The instructor or student obtains relative abundance (and mass) of each of the chlorine isotopes by holding the cursor on the top of each peak. Then, the instructor illustrates the method of calculating the atomic mass of chlorine from mass-spectral data.

In a homework assignment, students calculate atomic weights for several elements using mass-spectral data. The NIST WebBook contains this data for a limited number of uncombined polyisotopic elements including the inert gases krypton (five significant isotopes) and xenon (nine significant isotopes). Students determine the atomic masses of several metals from the mass spectra of some of their volatile compounds. Numerous metal–carbonyl compounds $[M(CO)_x]$ fragment in the mass spectrometer by loss of carbon monoxide ligands, which results in spectra consisting of clusters of peaks representing the various isotopes. By considering only the peaks associated with the metal-isotope ions, students calculate an accurate atomic weight. The spectra of compounds like $Cr(CO)_6$, $Mo(CO)_6$, $W(CO)_6$, $Fe(CO)_5$, and $Ni(CO)_4$ work well. Several volatile alkyl– and aryl–metal compounds fragment in the mass spectrometer by loss of alkyl or aryl radicals. Interesting examples include dimethylmercury, tetramethyllead and tetraphenyltin. The hazards associated with some of these substances preclude their consideration for laboratory use in an undergraduate setting. Use of internet-based data, however, allows even extremely hazardous substances to be considered.

Conclusion

Mass spectrometry used in the first semester of general chemistry enhances the communication of fundamental concepts like isotopes and atomic weights. For circumstances that preclude hands-on use of a mass spectrometer by general chemistry students, the Internet provides interactive mass-spectral data that encourages active learning. The use of Internet-based mass-spectral data also allows the consideration of highly toxic compounds that general chemistry students should never handle.

References and Notes

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