Letters

Levels of Description in Chemistry

I very much welcome William Jensen's series of articles (*1*) in which he stresses the importance of recognizing that there are three levels of description in chemistry. These are exemplified by:

1. Hydrogen is a colorless, light, inflammable gas; diamond is a colorless, hard, crystalline solid.
2. Hydrogen comprises H_2 molecules; a crystal of diamond comprises carbon atoms held together in a continuous framework.
3. Hydrogen molecules comprise two singly charged nuclei held together by two electrons; a crystal of diamond comprises a continuous array of C^{4+} cores held together by four times as many electrons.

Failure to keep these levels distinct, and to present chemistry in the logical order $1 \rightarrow 2 \rightarrow 3$, underlies many of the problems in chemical education today. For example, many students become proficient at levels 2 and 3 without being able to make connections with level 1 (*2*).

I am uneasy, however, about Jensen's terminology. He calls the first level "molar", as this is the etymological counterpart of "molecular" (Latin *moles*, large mass; *molecula*, small mass). However, "molar' has come to have a technical meaning in chemistry, as in "molar mass" and "molar volume" (*3*). I accordingly prefer the term "bulk" (*2*).

For level 2 Jensen adopts "molecular". He argues against the use of "atomic" on the ground that, at level 3, atoms do not exist in molecules. However, this breaks his own rule about keeping the levels distinct. Within level 2 one can talk about atoms in molecules, and this description is very useful. It is in any case possible to recover the concept of an atom in a molecule at level 3 if one allows atoms to be distorted (*4*). Ions can be regarded as charged atoms (*5, 6*).

A problem with "molecular" is that it is an inappropriate term for framework substances like copper, sodium chloride, and diamond. These are *nonmolecular* in the etymological sense of "molecular" (*6*). Jensen himself has referred to the "degree of nonmolecularity" of substances (*7*). For these reasons I prefer to designate level 2 as "atomic" (*2*).

Finally, Jensen refers to level 3 as "electrical". The problem with this is that there are two levels of description in electricity, macroscopic and microscopic, and "electrical" is commonly used for the former. For example, engineers distinguish between "electrical engineering" and "electronic engineering". For level 3 I use "electronic" or "nuclear" as appropriate (*2*).

I hope that these comments will not detract from the main thesis of Jensen's articles, which is singularly important.

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The author replies:

My decision to use the adjectives "molar", "molecular", and "electrical" to describe the three levels of chemical discourse was based solely on historical considerations and was designed to underscore the parallelism between the historical development of chemistry, outlined in Lecture III, and its current logical structure, outlined in Lecture I. As amply documented in the third lecture, the meanings that I attached to each of these terms accurately reflect the conceptual standpoints

Correction

The Literature Cited section was unfortunately omitted from the October 1999 NSF Highlights column, "Organic Chemistry Course Development in a Forensic Science Program: Use of FT-NMR" by Ronald Callahan, Lawrence Kobilinsky and Robert Rothchild (*J. Chem. Educ.* 1999, *76*, 1332–1333). The references are listed below.

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intended by the scientists who originally introduced them—the term "molar" in the late 19th century, the term "molecular" in the late 18th and early 19th centuries, and the phrase "electrical theory of matter" in the early 20th century. The history of nomenclature shows that it is virtually impossible to devise a terminology that is acceptable to everyone. If one restricts oneself to common Latin and Greek word roots, it is also increasingly impossible to come up with terms that have not been previously used for other purposes. These problems are present not only in my terminology but also in the alternatives proposed by Dr. Nelson.

Take, for example, the term "bulk". This is used in at least two ways in the technical literature. In the first case, it refers to the size of a sample as measured by its volume, or more specifically to changes in that volume in response to changes in mass (as in solution bulk or bulking), applied stress (as in bulk modulus), etc. (*1, 2*). In the second case, it refers to the major portion of a sample, independent of its overall size, as in bulk phase properties versus surface properties (*3*) or the bulk structure of a solid versus its surface structure (*4*). Here "bulk phase" refers to a level 1 description, whereas "bulk structure" refers to a level 2 description. In none of these cases does the term bulk function as a synonym for the term macroscopic.

Indeed, at level 1 chemists are not interested in "bulk" properties, which depend on sample size or volume, but rather in size-independent or intensive properties. These are usually measured in terms of the property value per mole, such as molar heat capacity, molar volume, molar polarization, molar conductivity, molar refraction, molar absorptivity, etc. I can't think of a better term than "molar" to describe that level of chemical discourse at which chemists are primarily interested in the measurement and correlation of molar properties. While it is true that chemists have made the original term more specific in order to intercompare chemically equivalent samples of different substances, this is a logical refinement rather than a contradiction of the more general usage employed in Lecture I. The unfortunate fact that the term "molar" is also used for a concentration unit conflicts as much with the concept of molar properties used in physical chemistry as it does with my more general usage, since the molar concentration of a solution does not measure its concentration per mole.

Likewise, Nelson's suggestion that the term "electrical" should be used at level 1 and the term "electronic" at level 3 does not stand up on closer scrutiny. Examination of a dozen materials science and solid state physics texts in my office revealed that they were divided roughly half and half between those that talked about the electrical properties of solids and those that talked about their electronic properties (*5*). In each case, the chapters in question intermixed models from all three levels of discourse. The true distinction between these two terms is not that of macroscopic versus microscopic but rather that of all possible electrical interactions versus those which deal solely with the electrons. At level 3 we talk about electrical forces between electrons and nuclei and not about electronic forces. The electrical potential energy of a molecule is the sum of both its electronic energy and its nuclear–nuclear repulsion energy, etc. (*6*).

Finally, at level 2, I would argue that the adjective "molecular" is a far more flexible term for describing the wide variety of entities found at this level than is the term "atom" and certainly does not carry the same metaphysical baggage. I agree with Nelson that the term atom is indispensable if one is teaching chemistry in the historical order 1 → 2 → 3, since, in the absence of level 3, one cannot describe level 2 without this term. However, once the student reaches level 3, I revisit the term and point out its ambiguity when looked at from the standpoint of the sequence 3 → 2 → 1, as is done in most books dealing with quantum mechanics. It is precisely because of this ontological ambiguity that I feel that the term atom, however necessary from a historical and pedagogical view, should not be used to describe a fundamental level of chemical discourse.

As for the term "nonmolecular", used in some of my earlier papers, I have now abandoned this term for the reasons given by Nelson and instead use the term "infinitely-extended structure" or, better yet, the terms "infinite framework polymer", "infinite layer polymer", and "infinite chain polymer." In keeping with these terms, I now talk about the degree of polymerization or catenation rather than the degree of nonmolecularity. This extension of polymer nomenclature to inorganic crystals was recommended more than 50 years ago by various polymer chemists (*7, 8*). Though I am sure that some chemists, who are accustomed to a far more narrow use of the term, will object, this broader usage is certainly in keeping with Berzelius's original intent when he coined the term in 1832.

Understandably Dr. Nelson and I are each enamored of our own particular terminology. One reason for introducing the labels "level 1", "level 2", and "level 3" was to provide a neutral alternative to more specific adjectives. It is a matter of a simple sentence to translate between one set of adjectives and another. I don't think there is much chance of confusion with these multiple choices and hence no good reason for being overly pedantic. In the end, individuals will use whatever adjectives appeal to them the most (or, more likely, they will simply ignore the whole thing). I thank Dr. Nelson for his kind and thoughtful comments and hope that our exchange will stimulate further discussion of these questions among chemical educators.

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Inexpensive Variable Pathlength Cells for Discovery-Based Investigation of the Beer–Lambert Law

In a recent article, Stewart and Sommer (*1*) suggest using acrylic or polycarbonate spacers to reduce the pathlength of 1-cm cuvettes in discovery-based investigations of the Beer–Lambert law. For several years, I have used similar experiments based on the work of Ricci et al. (*2*), but have used glass spacers to reduce pathlengths. These are quite inexpensive (for under $5.00, the staff at a local hardware cut 100 or so from scrap glass to my specifications) and of uniform thickness; they do not scratch easily, are essentially inert chemically, and give excellent results with a dual-beam spectrophotometer using equal numbers of spacers in both sample and reference cells (Fig. 1 illustrates typical results). The only disadvantage of glass is the sharp edges left after cutting; these can easily be removed with fine emery paper.

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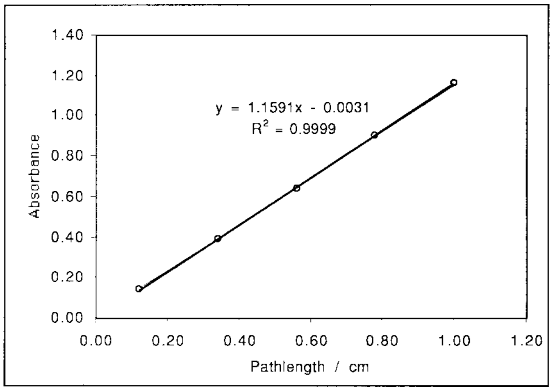
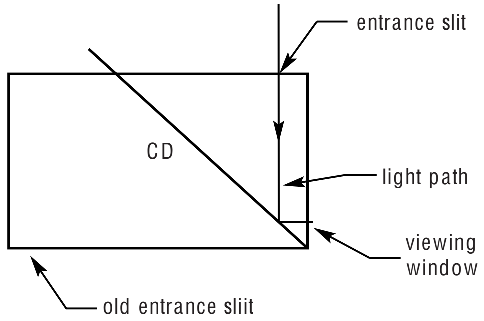


Figure 1. Plot of solution absorbance vs pathlength, using glass spacers. The least-squares fit equation and R^2 value are included. The absorbance was measured with a Shimadzu UV 260 dual-beam spectrophotometer at 470 nm for 0.00352 M I_2 in 0.00941 M KI.

CD Spectroscope

In using the *JCE* Classroom Activity #12, CD Light: An Introduction to Spectroscopy, one of my students, Elizabeth Blaisdell, found an interesting variation in the construction of the CD Spectroscope.



She made the box with CD and found it would not sit on a table. She proceeded to flip the box over, added an entrance slit of the same size above the viewing window on the new top of the box, and then repositioned the CD to fit into the edge of the box closest to the viewing window. The box now lies flat on a table and can still hold a petri dish, and the images shown through the viewing window are twofold. There are two spectra, the first- and second-order spectra, but the spectrum closest to the viewing window is enlarged to give a more detailed image. The observations are more clearly made and detailed. What a wonderful discovery!

Thank you for allowing me to share this.

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About Letters to the Editor

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