Commentary

Visualizing Chemistry

by Richard N. Zare

When my youngest daughter Rachel was a junior in high school, she brought home some stiff but flexible wire loops and a large collection of beads. Her homework assignment was to build a model of an atom, such as the gold atom with 79 electrons, and bring it back to school the next week. Evidently, Rachel's teacher wanted her to string the beads on the wire strands and create some model that would look similar to the logo made famous by the U.S. Atomic Energy Commission. The teacher told Rachel to ask a parent for help, which would ultimately prove to be my daughter's undoing. When presented with this problem, I foolishly convinced Rachel to make instead a model of the hydrogen atom, which meant that we discarded the beads and wire loops in favor of a heavy but tiny ball bearing that was placed in the middle of a spherical wad of cotton that got wispier and wispier as the periphery was approached.

I was delighted with this teachable moment. I explained to Rachel that the model we had constructed really did not do justice to the hydrogen atom. To mimic the hydrogen atom the nucleus needed to be so much smaller and denser but this construction was the best I knew how to do. I went on that what was important was not the weights of the cotton relative to the ball bearing but the opposite charges on the two. I explained that electrostatics rather than gravity is what dominated the world of chemistry on this scale. I enthusiastically babbled on about not knowing exactly where the electron was, hence the cotton electron cloud. I offered that if Rachel was interested we could next build together a hydrogen molecule.

As you probably already guessed, the teacher was not impressed. Just the opposite occurred. Rachel's teacher was unable to recognize this object as anything resembling an atom. Consequently, my youngest daughter received a failing grade for this homework assignment. Poor Rachel was unable to defend her model. The teacher remarked that it was no challenge whatsoever to make a hydrogen atom containing only one electron, which was supposed to be represented by just one bead. Seldom again would Rachel ask her father about anything involving chemistry that year. A painful parent-teacher conference never repaired the damage, although I learned an important lesson about communicating at the proper level.

Since that incident, I have wondered about the various models we use in chemistry to represent highly complex phenomena. To me, models are essential. The truth is that I think in terms of them, even though sometimes what I do looks highly mathematical. From what I can tell, most chemists are the same way. Chemists are highly visual people who want to "see" chemistry and to picture molecules and how chemical transformations happen. Yet how we depict the structure of a molecule has an amazing number of variations. We draw structures on flat paper, which is intrinsically two-dimensional, and yet one of the distinguishing features of chemistry is its three-dimensional architecture. We have various tricks for indicating that fact, which often confuses the beginning student. In addition, we use all types of shorthand for the nature of bonding, from dot structures, to single, double, and triple lines, to curves (bent bonds), to blobby molecular orbitals, to electron density maps. We have ball-and-stick models and space-filling models. In some advanced work we even have the ability with computers to experience in a tactile way the force field that some probe would be in if it were brought up to a molecule at some particular distance. These abstract representations are taken as part of the stock in trade of our profession. Often we do not give these matters much additional thought, even though we know how unobvious, if not overwhelmingly formidable, these models can appear to the uninitiated.

We need to celebrate more our model making. We are living in an information technology revolution that can be compared historically to Gutenberg's invention of moveable type. That invention took publication from an exclusive activity of a few (mostly monks in cloisters) to the many, resulting in a dramatic increase in the dissemination of the written word. It was during that time that monks also prepared illuminated manuscripts containing glorious pictures, often using pounded gold leaf. Thanks again to the information technology revolution today all chemists can also illustrate their own manuscripts, even if they have only modest artistic talents. Do not underestimate the power of kinetic art; we also have the ability to make arresting animations. For an example, see the animations and movies that Profes-

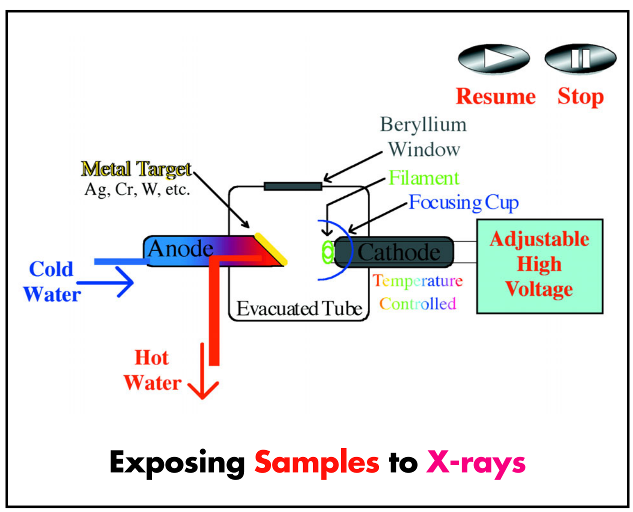

Figure 1. Single frame from an animated schematic diagram of an X-ray source used to initiate X-ray absorption or fluorescence. The animation is available at *http://www.shsu.edu/~chm_tgc/sounds/XAS.mov.*[1] Courtesy Thomas G. Chasteen.

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sor T. G. Chasteen has prepared and kindly made available to all of us; a snapshot from one of these appears as Figure 1.[1] I want to emphasize the importance of graphical material in telling our story of what we do, not only to each other, but also to those outside our field. Pictures seldom can capture all the subtle nuances of a model, but good pictures and movie clips are not only what are best remembered, they also often enable us to take the next steps in both teaching and research. In addition to being writers, we are now also illustrators and even movie producers. We must learn to use this power to communicate better what chemistry is all about.

Note

1. This is a snapshot from an animated sequence at *http://www.shsu.edu/~chm_tgc/sounds/sound.html*. It is one of many QuickTime, Flash, or GIF animations made available by Thomas G. Chasteen, Sam Houston State University, Huntsville, TX 77341-2117; *chm_tgc@shsu.edu*.

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