

Thoughts on Aesthetics and Visualization in Chemistry

Roald Hoffmann

Pleasure is constructed by human beings out of anything they do – in the best and worst of circumstances. I remember in the months after the war (my war, World War II), what fun there was in going with a group of boys and girls into a bombed-out house, the stairs partially collapsed, and sifting through the littered debris (treasures to us) of those who had lived there before. Or exploring a bunker, despite its pervasive smell of excrement. Who knows, one might find a bullet, get the powder out of it, set that on fire.

In Ithaca, in a definitely not bombed out laboratory, a graduate student has been trying still another solvent to get that Michael addition to go. It refuses, and she is afraid to ask her advisor for still another suggestion; he had made two (neither worked), and it's her research after all. So she tries again – for that is the fate of graduate students – leaving the solution to cool overnight. In the morning there are lime-green crystals. Hard sought, they are immediately beautified. And the research plan that led to them is imbued, *ex post facto*, with beauty.

Beauty is built out of individual pleasure around an object or idea. It may be personal, but gains in strength when it is shared with others. This will not pass Kantian muster, but I think it is the key to including in the aesthetic universe artifacts and human actions that are not the 'high' art central to typical philosophical discussions of beauty. Such as the stuff of chemistry. The components of the aesthetic transaction are the object or idea, the human being who created it, and the one who contemplates it, the two linked in separate, yet intense, pleasurable contemplation. Or perhaps action. And after Goya and the 20th century, the scope of pleasure widens to include not just that which makes us smile.

Chemistry, the art, craft, business, and now science of substances and their transformations, is today paralleled at every step by hard-won microscopic knowledge of molecules and their reactions. Chemistry is also human labor – even the calculational chemistry that some of my colleagues in theory say will make for an odorless future, even that requires much (computer) work. The human beings who are drawn to chemistry, in both its analytical and synthetic parts, construct compounds and meaning. And imbue the sub-

stances, and the little pictograms we draw of them, with intimations of beauty. Why? Because building a pleasurable rationale for hard labor is a psychological necessity. And because we naturally seek beauty, as we seek good. At least that matches Kant.

The process is inherently messy. To make things harder, in science aesthetic discourse is out of bounds in the published record. No matter, little joys cannot be suppressed, they emerge in group meetings and banter. Eventually philosophers (and reflective practitioners) see there is something to analyze. Just as scientists in their daily practice, we do so by categorization, a time-honored and productive scholarly process. We glean molecular beauty by taking it apart. As we do so, it's important not to get too upset by the irrational element in the assignation of beauty by supposedly logical people. So they make up a reason for this step in a synthesis being elegant, not because it is, but because it worked after long failure... So they don't respect categories; they anthropomorphize, they talk of a compound as if it were a molecule, and they draw a model but talk about a molecule. I would say that a lot of creation in science takes place by thinking in almost circular ways, transgressing categories and logical definitions. In a way metaphors are just that.

Someone asked me to discuss in print the way chemistry is written. I wound up talking so much about how it is drawn that I had to title the article "Writing (and drawing) chemistry". Why all stress on images in both alchemy and chemistry? The transformations wrought by metallurgists, by glass and dye makers were truly awesome. I think of a wool cloth drawn out of a yellowish fermented urine solution of indigo, turning blue before our eyes. I think of dull earths smelted into bronze, of a red crust forming on mercury under the action of a burning lens. These emblems of change were adopted by philosophies of transformation when they needed an emblem with which to get into peoples' minds. And then, lo and behold, the philosophies themselves were co-opted by chemistry. Alchemy was a unique cultural experiment – the imagery of real chemistry (and its smells, its sounds, the infernal and necessary heat), that it mattered in whose hands something was done (still, in this age of reproducibility a concern to synthetic organic chemistry), essential to its function.

In time, visualization via models enters chemistry, as an inevitable corollary of the macro/micro motion that confusingly and productively mixes in the minds of modern chemists. Layers of iconic and symbolic representation of molecules mediate our struggle to propel ourselves into understanding why out of that blue solution comes a lime green precipitate. We understand, not just by cogitation, but through drawings of molecular models and orbitals, on blackboards and restaurant napkins.

The other impulse toward visualization comes from the success of the architectural way of thinking about structure and building in chemistry.

Molecules are classical objects, even as they are in small ceaseless motions. And they are also quantum objects, in their spectra. Still classical thinking will get you a long way – think of today's excitement in supramolecular chemistry. The communication of molecules' architectonic essence by little iconic drawings (rather than photographs or etchings), and by ball and stick models, is of proven value – remember this year marks half a century since the Watson and Crick paper. They didn't synthesize DNA, they reasoned out its structure, almost willing a model into being.

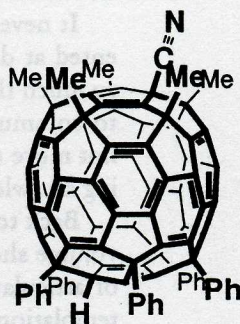
It never ceases to amaze me how a community of people who are not talented at drawing, nor trained to do so, manages to communicate faultlessly so much three-dimensional information. And... that people who have learned to communicate visually in such a variety of artistic styles – chemists – are not more tolerant of expressionist and abstract artistic ways of communicating knowledge and emotion.

Back to aesthetics: clearly a motive force in chemistry, as the essays in this volume show. Though, as I have tried to argue, shaped out of the psychology of articulating pleasure in achieved labor as much as from disinterested contemplation. There are dangers, however, in canonizing aesthetic motivation. The aesthetic innate in us is incomplete – we have somehow evolved to favor simplicity. This is not all good, for with that inbred love of the simple comes... prejudice and a falling for demagoguery, and for advertising. These cater to that love for the simple and pure in us. The beeline that cubane and a simple melody have into our soul, compared to the struggle that ribonuclease and a composition by György Ligeti has to be admired, are connected, I feel, to reductionist fantasies of physicists that beautiful (read 'simple') equations must be true.

My other concern about aesthetics driving science is that I'm worried that it leads, in the context of self-justification, to talking down utility and ethical concerns. It seems to me that modern science, and chemistry in particular, has lost a little of the romantic but ultimately necessary idea that one goal of science is ameliorative – as Peter Medawar has said: to leave the world a little, just a little better place than the way we found it. I occasionally get the feeling that scientists (and artists) sometimes use aesthetic value as an excuse not to think about ethics.

I recently saw a beautiful molecule in the literature. The authors, E. Nakamura and collaborators (Nakamura, E.; Tahara, K.; Matsuo, Y.; Sawamura, M.: 2003, 'Synthesis, Structure, and Aromaticity of a Hoop-Shaped Cyclic Benzenoid [10]Cyclophenacene', *Journal of the American Chemical Society*, 125 (10), 2834-35), explained by way of introduction how they and others had long sought to make 'hoop' type compounds, in which there is delocalization of electrons around a finite cylinder. Note the muddle of compounds (materials), molecules, and models in my, and their, language. Remarkably,

they gained access to a hoop geometry, not at all in the way everyone had logically thought of trying, but by the unexpected desymmetrization of the beauty (Platonic and Brazilian) of buckminsterfullerene. On addition of 12 groups of four different kinds (five methyls, five phenyls, a cyano, and a hydrogen!), one was left with a delocalized band of atoms, still embedded in a C_{60} framework (see structure below). Not the archetype freestanding (rolling) hoop, but still clearly a hoop. Neat, destroying one beauty to make another one.



Beauty does not reside in simplicity. Nor in complexity, per se. For a molecule or a song, for a ceramic vase or a play, beauty is created out of the labor of human hands and minds. It is to be found, precarious, at some tense edge where symmetry and asymmetry, simplicity and complexity, order and chaos, contend.

Roald Hoffmann:

*Department of Chemistry and Chemical Biology, Cornell University,
Baker Laboratory, Ithaca, NY 14853-1301, U.S.A.*