published in modified form in:
Peter Weibel & Ljiljana Fruk (eds.): *Molecular Aesthetics*, Cambridge, MA: MIT Press, 2013, pp. 155-161.

Molecular Aesthetics: Blind Alleys and Fertile Soils

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1. Introduction

Since the advent of synthetic organic chemistry in the mid-19th century, chemists have frequently pointed out the creativity, imagination, and aesthetic inspiration required for chemical synthesis (Root-Bernstein 2003, Jacobs 2006, chaps. III.4-5). Most famously Marcelin Berthelot (1860) compared the chemo-synthetic work to that of the 'arts' because, like artists and unlike other natural scientists, chemists create their own objects of study on a regular basis. Although modern commentators tend to overlook the ambiguity of the term 'arts', which in the 19th century did not mean so much the fine arts but crafts and engineering as opposed to the sciences, the efforts by chemists to relate their science to the formative arts are undeniable.

Compared to these ongoing efforts, which are frequently part of a helpless strategy to popularize chemistry, serious aesthetic research is still underdeveloped. While classical anthologies on aesthetics in science have largely focused on mathematical physics – following an almost campaign-like advance by Paul Dirac, Eugene Wigner, Richard Feynman, Werner Heisenberg and others in the 1960s and early 1970s (Stevens 2003) – chemistry stands in isolation. Before 2000, only a handful of papers on chemistry appeared in aesthetics journals (Hoffmann 1990, Hargittai & Hargittai 1994, Schummer 1995, Root-Bernstein 1996); the first, and thus far still only, collection of papers on aesthetics in chemistry was not published before 2003, which incidentally had an accompanying part of artistic contributions on "Chemistry in Art" (Specter & Schummer 2003).

In contrast to the wide opportunities for aesthetic studies of chemistry, particularly on the role of aesthetic values in the practice of experimentation and theory building (Ball 2005, Schummer et al. 2009), the dominant focus has been on the beauty of molecules, like that of the present volume. Indeed, chemists aesthetically favor molecules that are either symmetrical or look like ordinary objects. That double-preference seems to echo the formative arts in which both geometrical abstraction and imitation of nature have a long tradition.

In the following I will scrutinize, first, if molecules can be objects of aesthetics at all; second, if symmetry is a useful aesthetic criterion for beauty; and, third, explore the hidden aesthetic potential behind molecules that "look" like ordinary objects. In order to do so it is necessary to start with the oldest molecular theory, which happened to be built on aesthetic ideas and which is frequently referred to in contemporary claims about the beauty of chemical products.

2. Plato's molecular aesthetics and the problematic status of molecules

In the still ongoing dispute over the priority of the aesthetics of art versus the aesthetics of nature, Plato held an early radical view: Because the formative artists only try to imitate nature, and because material nature is only an imitation of the true ideas of nature, their artworks are of limited, third-class value (e.g., *Sophistes*, 266 c-d). Moreover, if artists try to arrange their imitations of nature so as to cater to the perspective and aesthetic views of the beholder - when they, for instance, try to compensate for perspectival distortions by the human eye - they are cheating on nature (*Sophistes*, 236 b). Their disregard for the truth of nature disqualifies the beauty of their products. Thus, whoever seeks support for molecular aesthetics in Plato should be aware that he would have harshly criticized the artistic production of molecules and even more so their colorful graphic representations.

While he grumbled about the formative arts and artists, Plato praised nature as the embodiment of beauty in his dialogue *Timaeus*. From the presupposed beauty of the ultimate components of nature he tried to infer their shape, using aesthetic criteria as guidelines for theoretical knowledge (*Timaeus,* 53e). Starting with simple triangles he built up the famous series of regular polyhedra (the so-called Platonic solids: tetrahedron, octahedron, cube, icosahedron, see Figure 1), which should correspond to the four elements fire, air, earth, and water. He believed that the polyhedra are invisibly small and react with each other so as to rearrange their triangle components to form different polyhedra. Remarkably, this oldest molecular theory of chemical reactions (Rex 1989) was developed on aesthetic grounds.

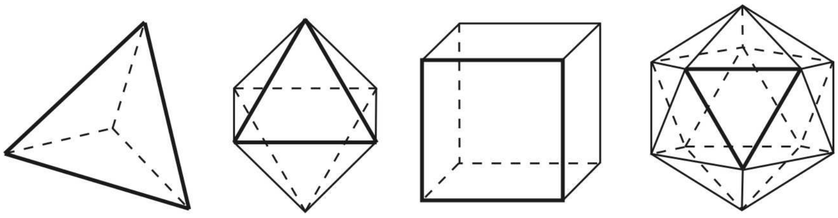

Figure 1: The Platonic solids: tetrahedron, octahedron, icosahedron and cube, representing the ancient elements fire, air, earth and water.

The molecular entities that Plato devised as the embodiment of natural beauty had, philosophically speaking, a hypothetical status. Similar to today's chemical molecules, they were neither objects of human sensation nor merely intellectual ideas, but supposedly real entities, devised by intellectual reasoning but being beyond the scope sensation. They inherited their beauty from the underlying geometrical ideas, which for Plato were the true candidates of beauty. The hypothetical status still today makes it difficult to treat molecules by any of the available aesthetic theories, which are tailored either for perceptible objects, such as sculptures or paintings, or for intellectual object, such as ideas or concepts embodied by particular artworks.

Although some chemists, particularly organic chemists, deal with molecules in their daily practice as if they were ordinary objects, they are, according to the best of our physical and chemical knowledge, quite complex theoretical entities. Strictly speaking, the talk of molecules as stable and isolated classical entities makes sense only within the scope of a model approach that disregards most of quantum mechanics, reduces the interactions between atoms to the ideal of covalent bonds, and disregards all intermolecular interactions (Schummer 1998). Popular and useful as it is in most of organic chemistry, that approach badly fails with metals, salts and, for most cases, even with simple substances like water. Neither standard spectroscopic measurements, such as infrared (IR) or nuclear magnetic resonance (NMR) spectroscopy, nor diffraction methods by x-rays, neutrons or other particles, nor electron microscopies and the more recent scanning probe spectroscopies (STS) simply provide direct images of molecules. Unlike widespread popularizations of chemistry and nanotechnology, measurement data must be heavily processed to yield the cheerful molecular images that decorate book covers and magazine titles (Pitt 2006, Schummer 2009, chap. 11)

Thus, similar to Plato's tiny polyhedra, today's molecules resist standard aesthetic appreciation for ontological and epistemological reasons. Those who ignore the issues typically confuse molecules with molecular representations and models, a standard distinction in the epistemology of science. If, on the other hand, one wishes to solve the problem with reference to Plato's own theory, it becomes difficult to avoid the conclusion that the artistic production of molecules, like that of other imitating arts, is at best an obsolete play.

3. Mathematical symmetry as a questionable aesthetic criterion

Among the molecules chemists have praised for their beauty, those with high mathematical symmetry stand out. In fact several chemists have confessed that the aesthetic appreciation has been a major impetus for their synthetic research of symmetrical molecules (Grahn 1981, de Meijere 1982, Hoffmann 1990, Hargittai 2000, pp. 419f.). It should be noted that mathematical symmetry is largely independent of whether a molecule is considered a classical or quantum-chemical entity and thus applies to molecular models, like ball-and-stick models used in educational contexts, and quantum-chemical molecules alike. Thus, symmetry appears to be an ideal property to avoid the frequent epistemological confusion between molecules and molecular models. It is a mathematical description of geometrical forms according to the invariance with regard to certain transformations, such as reflection on a mirror plane, rotation around an axis at a certain angle, or lateral translation by a certain distance. In this approach, the higher the symmetry, the simpler is the form, which makes symmetry a measure of mathematical simplicity.

However it is questionable if mathematical symmetry is a useful aesthetic criterion for beauty (Schummer 2006a). While in ancient Greek aesthetics, particularly following the works of the sculptor Polykleitos, symmetry played a dominant role, its meaning was totally different from today's. It described balanced proportions between different lengths, such as between the size of the head and the size of the body or the whole of a sculpture, or between opposed compositional elements, such as between static and dynamic parts. The measures of balanced proportions were not taken from mathematics but from natural models like the perfect human body. Contrary to the still prevalent popularization of physics, mathematical symmetry was totally unknown in antiquity and thus played no role in classical aesthetics. Instead it was developed only in 19th-century mineralogy as an approach to classify crystals (Scholz 1989).

Thus, if chemists praise the beauty of their symmetrical molecules, they find little support in classical aesthetics, except in Plato who, of course, considered the 'Platonic bodies', which happen to be highly symmetrical in the modern sense, beautiful. Yet, for him only the mathematical ideas behind them were the true candidates of beauty, whereas the manufacturing of corresponding material models, either of molecular or human size, would have been but the proliferation of second-grade material imitations.

Plato's aesthetic preferences of the regular polyhedra was probably based on epistemic criteria, here mathematical simplicity in term of recurrent angles and edges, which allowed him to identify beauty with truth. However, with the advent of modern aesthetics (and epistemology) both became disentangled. In particular Kant pointed out that people tend to confuse epistemic satisfaction, resulting from easily grasping or recognizing something, with aesthetic pleasure (Kant 1799, S. 70f, 277f). While the latter resists simple explanation and is usually enduring for a while, symmetrical objects please only for a short moment and immediately become boring once their mathematical construction has been understood.

> "All stiff regularity (such as borders on mathematical regularity) is inherently repugnant to taste, in that the contemplation of it affords us no lasting entertainment and […] causes boredom." (Kant 1799, S. 7)

If mathematical symmetry were the ideal of beauty, classical artists striving for beauty would have produced nothing else than perfect spheres, which actually bear the highest degree of symmetry of all bodies. Of course they did not do so. Instead, as many art theorists have pointed out, mathematical symmetry has played an important role in art only as the counterpart to disorder or as a kind of background for highlighting symmetry breaks, from the use of ornaments in architecture to minimal art – which follows the antique idea of artistic symmetry as a balance between order and disorder.

The preference of mathematical symmetry, and its confusion with beauty, can even seriously mislead scientific research. Indeed Plato's idea that Nature favors simple regular forms was disproved in a theoretical study of 1937 by Hermann A. Jahn and Edward Teller (Jahn & Teller 1937). They showed that under certain conditions, which are actually quite common, regular molecular polyhedra are instable compared to distorted polyhedra (in which electronic energy states are split such that lower states can be populated). More recently it became also obvious that their fondness of symmetry has made chemists blind for an enormous technological potential that materials scientists are harvesting instead. While synthetic chemists have been producing purified substances that approach the ideal crystal with perfect translational symmetry, materials scientists have explored impure materials, with dislocations and other crystallographic irregularities in the nanometer range, which has opened up an entirely new field of properties and which has recently been subsumed under the realm of nanotechnology. Against romantic ideas about the aesthetic guidance of science, the two cases illustrate that this can, but need not, go at the expense of both epistemic and technological goal achievement. In sum, mathematical symmetry is neither an aesthetic criterion for beauty, nor does it provide epistemological or technological guidance in chemistry.

4. Making molecules look like ordinary objects and the aesthetics of molecular representations

In addition to their fascination with symmetrical molecules, chemists have been particularly enthralled since the 1980s by molecules that 'look' like ordinary objects (e.g. Vögtle 1989). Because molecules are invisible, indeed the result of a model approach that reasonably applies only to certain substance classes (see above), it is rather a set of molecular images that have raised their fascination. These images are captivating because of their ambiguity. On the one hand they refer to entities in the molecular world; on the other hand they refer to objects of the ordinary world, like a basket with a handle, a wheel on an axis, or two interlocked links of a chain (Figure 2). From a classical chemical point of view, these two worlds are quite disparate and disconnected from each other, because all the molecular properties that chemists are interested in are just missing in ordinary objects and vice versa.

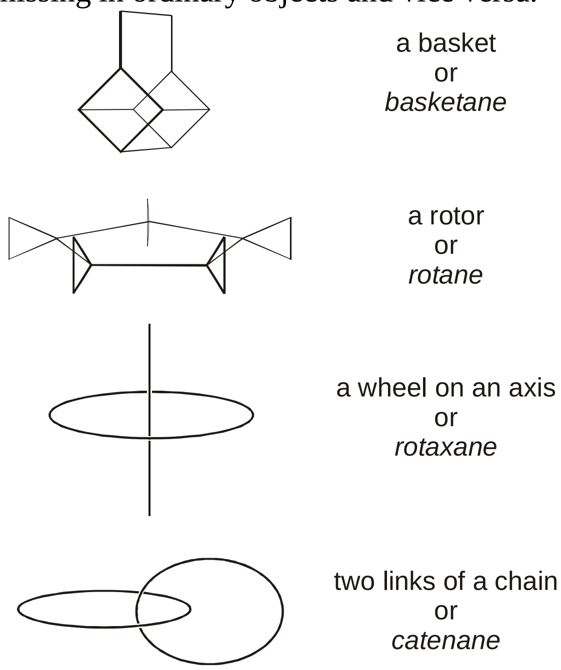

Figure 2: Molecular representations that look like ordinary objects.

However, owing to their ambiguity, the images connect these two worlds in a productive manner that stimulates the imagination of combining both worlds into one. One way to do so appeared in cartoons of little humans walking through and playing with molecules like ordinary objects (Figure 3). Another way was to reproduce by chemical means the ordinary world in miniature. Indeed, since the 1980s, chemists have imitated all kinds of ordinary world objects on the molecular level, from funny things like dogs and pigs to technological artifacts like gears, turnstiles, and elevators. They have developed a whole battery of molecular systems and devices with various mechanical and electrical functions, like molecular machines and circuits. The field thus inspired by the aesthetic phenomenon of ambiguous images came to be known as supramolecular chemistry and, more recently, as molecular nanotechnology (Balzani et al. 2003).

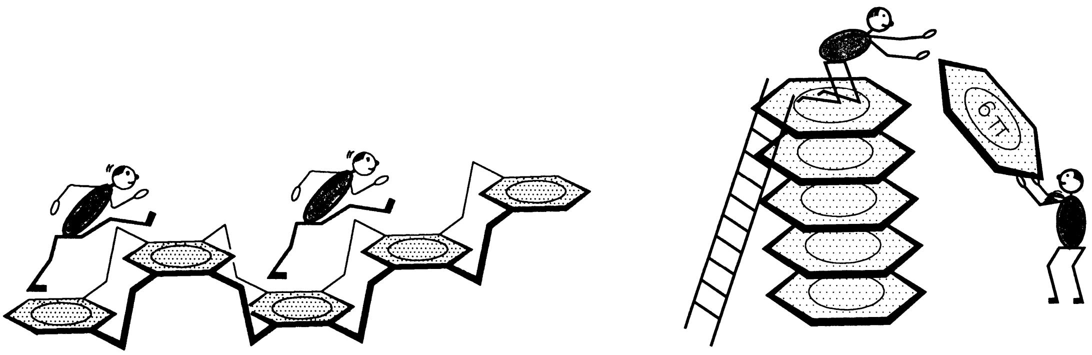

Figure 3. Cartoons from Vögtle 1989, pp. 5, 345 (modified versions from S. Misumi, first published in *Chemistry Today*, 78 [1977], p. 12, 22).

Umberto Eco's semiotic theory of aesthetics (Eco 1962/1989) is a useful approach to understand the aesthetic inspiration that has triggered the historical development (Schummer 2006b). Faced with ambiguous signs, the interpreter is prompted to lower the tension of ambiguity by developing new, potentially reconciling interpretations and by contemplating and revising the form of the signs. Indeed supramolecular chemists have not only tried to solve the ambiguity by reproducing the ordinary world on the molecular level, they have also developed a new chemical language of technomorph signs which they frequently use in combination with classical structural formulas. In accordance with Eco's aesthetic theory, this creates a new productive tension that calls for reinterpretation and semiotic revision as a reiterative process, which chemists perform by exploring further parts of the ordinary world on the molecular level and adjusting their sign language. In Eco's theory, the process eventually reveals more about the interpreters and their imagination than about the original signs. Estimated from the specific areas of the ordinary world that chemists have selected to imitate on the molecular level, chemists revealed a deep fascination with mechanical and electrical engineering.

5. Conclusions

Since the early 1980s chemists have repeatedly alluded to molecular aesthetics when praising molecules that either look like ordinary objects or that bear high degrees of mathematical symmetry. However, on a closer look, such aesthetic approaches face at least two serious conceptual obstacles. First, mathematical symmetry is a questionable aesthetic criterion that only through thoughtless popularization of science has been lumped together with the old artistic idea of symmetry. Second, and more important, molecules evade standard aesthetic theories because of their particular ontological status: they are neither simple empirical entities (but inaccessible by sense perception and thus cannot 'look' like something) nor mere conceptual entities or ideas to be judged by aesthetic values. If made accessible to the senses, it is not a molecule but a molecular representation – a model, a drawing, or a 3D-computer animation – that becomes the object of aesthetic judgment.

Thus, molecular aesthetics inevitably becomes aesthetics of molecular representations. Two options are possible. First, every now and then, when some funding is available or when the need to polish the public image of chemistry becomes particularly strong, we can launch a campaign to praise the beauty of the colorful images that chemists produce with the help of some hired artists. Second, we develop a serious research program in aesthetics that analyses aesthetic preferences and styles in the rich production of molecular representations. On the one hand, this opens up a huge field for cultural and visual studies of science by investigating the chemical practices of image production within a wider cultural context, thereby embedding chemistry into society at large. On the other, as has been illustrated in the previous section, we can look for cases in which aesthetic ideas have been the driving forces of research programs or even triggered entirely new fields, such as supramolecular chemistry, in order to establish the thesis that aesthetics is an inherent part of science.

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