Harmony of Forms and Processes
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ASPECTS OF MOLECULAR BEAUTY

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Abstract: *Molecules are objects of nature like a landscape, a plant, an animal or a human. Accordingly they may be beautiful, especially in the eyes of a chemist who works at his/her computer and constructs, inspects and understands molecular models. These models serve chemical thinking, experiments can be designed with much more certainty, molecular processes can be understood in more detail if we "see" our objects, i.e. we use more or less appropriate models reflecting the properties and action of the molecules. In this paper I discuss some aspects of molecular beauty and I must admit that my discussion is strongly biased. The reader will understand that I do like molecules, I enjoy work with them on the screen and presenting them in my lectures to laymen or to experts. I would share this feeling with artists and aesthetes, strongly believing that they may share my feelings upon inspection of colorful and rich in shape molecular models.*

1 INTRODUCTION

Molecules are part of Nature, like other macroscopic objects as landscapes, plants, animals or humans, thus a certain intrinsic beauty can be attributed to them. It should be stressed that beauty cannot be defined exactly, since it relies on personal taste, formed by education, experience and a variety of subjective feelings. As it is written on the WordNet (2008) “under beauty we mean the qualities that give pleasure to the senses”, while according to the Wikipedia (2008a) “beauty is a characteristic of a person, place, object or idea that provides a perceptual experience of pleasure, meaning or satisfaction”. The subjective experience of beauty often involves the interpretation of some entity as being in balance and harmony with nature, which may lead to feelings of attraction and emotional well-being. "Beauty is in the eye of the beholder" (Martin, 2007) or in other terms “beautiful is, what I do like”.

It is not surprising that the concept of molecular beauty does not meet consent. The famous chemist, Roald Hoffman (1990) discussed the beauty of molecules in terms of shape, utility, novelty, richness, decorative power and simplicity. In the following I focus on two further aspects, symmetry and dynamics, while I discuss richness in terms of complexity, which is an outstanding feature of molecular beauty. Molecular graphics is a valuable tool to provide graphic representations of molecular systems; accordingly, I illustrate my conclusions with some computer generated pictures.

2 SYMMETRY

Wikipedia (2008b) writes that symmetry is an “imprecise sense of harmonious or aesthetically-pleasing proportionality and balance; such that it reflects beauty or perfection. The second meaning is a precise and well-defined concept of balance or patterned self-similarity that can be demonstrated or proved according to the rules of geometry”, or another exact scientific discipline. This definition clearly allows consideration of symmetry as an aspect of molecular beauty, since molecular symmetry is an essential concept, which allows understanding and modeling a wide variety of molecular properties.

On Figure 1 I present two graphic models depicting symmetric chemical structures. The first represents simple symmetry, body centered cubic packing of atoms in a crystal. X-ray diffraction studies revealed that a variety of crystals, like halite (rock salt, NaCl), several metals (e.g. iron and tungsten), and alloys show this arrangement at the atomic level. The other model refers to the orthorhombic $CuInOPO_4$ crystal, where the stretched cubic lattice is formed by locally symmetric CuO_6-octahedra, which are connected by common edges. This way symmetry is combined with complexity, offering a sophisticated experience via inspection of the coloured graphic representation of the arrangement of atoms in the crystal.

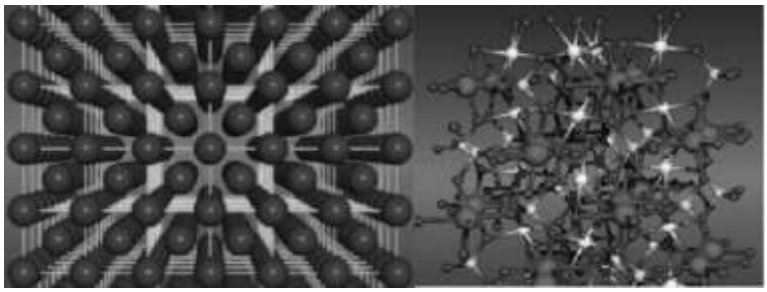

Figure 1: Simple symmetry: body centered cubic packing of atoms in a crystal (left), sophisticated symmetry: crystal structure of $CuInOPO_4$ (right) (after Immel, 2005).

3 COMPLEXITY

It seems that knowledge of function plays an important role in aesthetic appreciation. In the world of molecules complexity is one of the basic components of functionality, since in a broad sense complex molecules offer more opportunity to exert sophisticated function than simple ones. One example is that of proteins. These are complicated molecules with a special arrangement of atoms allowing accommodating smaller molecules and releasing them unchanged or split in parts by some functional groups within the crevice. Figure 2 shows the binding of a small molecule to a hollow crevice

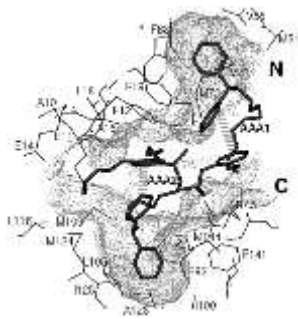

Figure 2: Binding of arylalkylamine molecules (AAA1 and AAA2) to the calmodulin crevice (Harmat et al., 2000).

of a protein, resulting in a biological response. Interaction of complex protein molecules with each other or with small molecules play an essential role in a variety of life processes, like enzyme action, immune response, muscle contraction, and so on. Functional beauty of proteins is manifested via graphical representation, which may be quite rich since beside shapes colors also play a role in the computer-generated image.

4 DYNAMISM

There is certain dynamism in the beautiful (Cohen, 2007). If this is true, a manifold of models showing action, variability or flexibility of a series of molecules, like in Figure 3, is certainly beautiful. Once again, this refers to functionality, since molecules provide more action if they are flexible and thus appropriate to adapt various conformations and interact with each other or with other molecules. Flexibility is a key factor in polymer function, drug design and other fields of molecular sciences. Dynamism allows the viewer an aesthetic experience in the form of a molecular movie (Molgraph3D, 2008).

Figure 3: Superimposed molecules (atoms and bonds represented by vertices and tubes, respectively) illustrating conformational flexibility.

Dynamism of molecules has been combined with dance and music in a work by Fekete-Kiss (2006) offering an example for the artistic representation of molecular concepts and thus bridging the gap between exact sciences and arts, or in other terms, between knowledge and emotion.

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