
Molecular Beauty

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What makes molecules beautiful? It may be their simplicity, a symmetrical structure. Or it may be their complexity, the richness of structural detail that is required for specific function. Sometimes the beauty of a molecule may be hidden, to be revealed only when its position in a sequence of transformations is made clear. Novelty, surprise, utility also play a role in molecular aesthetics, which is the subject of this contribution.

Recently my wife and I were on our way to Columbus, Ohio. After I settled on the airplane, I took out a manuscript I was working on – typical for the peripatetic obsessive chemist. Eva glanced over and asked, ‘What are you working on?’ I said: ‘Oh, on this beautiful molecule’. ‘What is it that makes some molecules look beautiful to you?’, she asked. I told her, at some length, with pictures. And her question prompted this exposition.

What follows is then an empirical inquiry into what one subculture of scientists, chemists, calls beauty. Without thinking about it, there are molecules that an individual chemist, or the community as a whole, considers to be the objects of aesthetic admiration. We will explore what such molecules are, and why they are said to be beautiful.

In the written discourse of scientists, in their prime and ritual form of communication, the periodical article, emotional descriptors, even ones as innocent as those indicating pleasure, are by and large eschewed. So it is not easy to find overt written assertions such as: ‘Look at this beautiful molecule X made’. One has to scan the journals for the work of the occasional courageous stylist, listen to the oral discourse of lectures, seminars or the give and take of a research group meeting, or look at the peripheral written record of letters of tenure evaluation, eulogies or award nominations. There, where the rhetorical setting seems to demand it, the scientist relaxes. And praises the beautiful molecule.

By virtue of not being comfortable in the official literature – in the journal article, the textbook or monograph – aesthetic judgments in chemistry, largely oral, acquire the character of folk literature. To the extent that the modern day subculture of chemists has not rationally explored the definition of beauty, these informal, subjective evaluations of aesthetic value may be inconsistent, even contradictory. They are subfield (organic chemistry, physical chemistry) dependent, much like the dialects, rituals or costumes of tribal groups. In fact the enterprise of excavating what beauty means in chemistry seems to me to have much of the nature of an anthropological investigation.

But this is not going to be your typical, seemingly detached critical analysis revealing with surgical irony

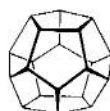
the naive concepts of beauty held by a supposedly sophisticated group of people. The honesty and intensity of the aesthetic response of chemists, when they allow themselves to express it, must be taken positively, as a clue to an unformulated good, as spiritual evidence, as a signpost to record, to empathise, to make connections with other aesthetic experiences.

Aesthetic judgments made by chemists about chemistry are perhaps more cognitively informed than aesthetic judgments in the arts (more on this below), which ensures that those judgments are jargon laden. But I am certain that people outside of chemistry can partake of what makes a chemist’s soul jump with pleasure at the sight of a certain molecule.¹ It is worth trying to see the motive force for all that intense, disinterested contemplation.

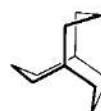
The shape of molecules

Let us begin with the obvious, which was not accessible to us until this century, namely *structure*. Molecules have a shape. They are not static at all, but always vibrating. Yet the average positions of the atoms define the shape of a molecule.

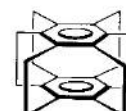
That geometry can be simple, or it can be exquisitely intricate. Structure 1 is a molecule with a simple shape, dodecahedrane. This $C_{20}H_{20}$ polyhedron (the polyhedron shows the carbons; at each vertex there is also a hydrogen radiating out) was first made in 1982 by Leo Paquette and his co-workers.^{2,3} It was a major synthetic achievement, many years in the making. The Platonic solid of dodecahedrane is simply beautiful and beautifully simple. Molecule 2 has been dubbed manxane by its makers, William Parker and his co-workers.⁴ Its shape resembles the coat of arms of the Isle of Man. And molecule 3 is superphane, synthesised by Virgil Boekelheide’s group.^{5,6} All are simple, symmetrical and devilishly hard to make.



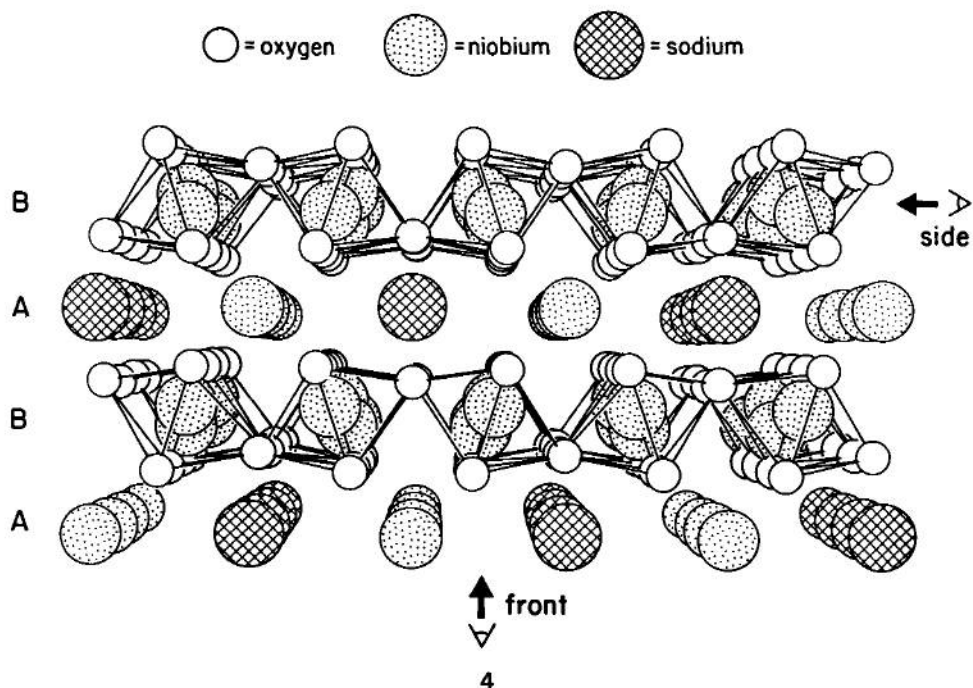
1



2



3



Let us try a structure whose beauty is a touch harder to appreciate. Arndt Simon, Tony Cheetham and their co-workers have recently made some inorganic compounds of the formula NaNb_3O_6 , $\text{NaNb}_3\text{O}_5\text{F}$ and $\text{Ca}_{0.75}\text{Nb}_3\text{O}_6$.⁷ These are not discrete molecules but extended structures, in which sodium, niobium and oxygen atoms run on in a small crystal, almost indefinitely. Structure 4 is one view of this truly super molecule.

Some conventions: the white balls are oxygens (O), the stippled ones niobium (Nb), the cross-hatched ones sodium (Na). The perspective shown chops out a chunk from the infinite solid, leaving it up to us to extend it, in our mind, in three dimensions. That takes practice.

Deconstruction aids construction. So let us take apart this structure to reveal its incredible beauty.

In drawing 4 we clearly see layers or slabs. One layer (marked A) is shown in structure 5. It contains only niobium and sodium atoms. The other layer, B (structure 6), is made up of niobium and oxygen atoms arranged in a seemingly complex kinked lattice-work. Let us take on this B layer first.

The building block of the slab is an octahedron of oxygens around a niobium. One such idealised unit is shown in drawing 7, in two views. In drawing 7a, lines (bonds) are drawn from the niobium to the nearest oxygen. In drawing 7b these lines are omitted, and instead the oxygens are connected up to form an octahedron. Which picture is right? which is the true one? Sorry – both are. Or, better said – neither is. Three dimensional molecular models, or their two dimensional portrayals, which is what we have before us, are abstractions of reality. There is no unique, privileged model of a molecule. Instead, there is an infinite variety of representations, each constructed to capture some aspect of the essence of the molecule. In drawing 7a the essence is deemed to lie in the chemical bonds, a pretty good choice. These are Nb–O; there are no O–O bonds. Yet portrayal 7b draws lines between the oxygens. This representation seeks after another essence, the polyhedral shapes hiding in the structure. Graphically, forcefully, drawing 7b communicates to us that there are octahedra in this structure.

You may wonder where these octahedra are in the

