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# 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

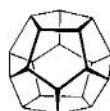
the naive concepts of beauty held by a supposedly sophisticated group of people. The honesty and intensity of the aesthetic response of chemists, when they allow themselves to express it, must be taken positively, as a clue to an unformulated good, as spiritual evidence, as a signpost to record, to empathise, 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.<sup>1</sup> It is worth trying to see the motive force for all that intense, disinterested contemplation.

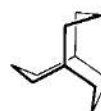
## The shape of molecules

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.

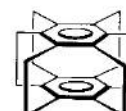
That geometry can be simple, or it can be exquisitely intricate. Structure 1 is a molecule with a simple shape, dodecahedrane. This  $C_{20}H_{20}$  polyhedron (the polyhedron shows the carbons; at each vertex there is also a hydrogen radiating out) was first made in 1982 by Leo Paquette and his co-workers.<sup>2,3</sup> 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.<sup>4</sup> Its shape resembles the coat of arms of the Isle of Man. And molecule 3 is superphane, synthesised by Virgil Boekelheide’s group.<sup>5,6</sup> All are simple, symmetrical and devilishly hard to make.



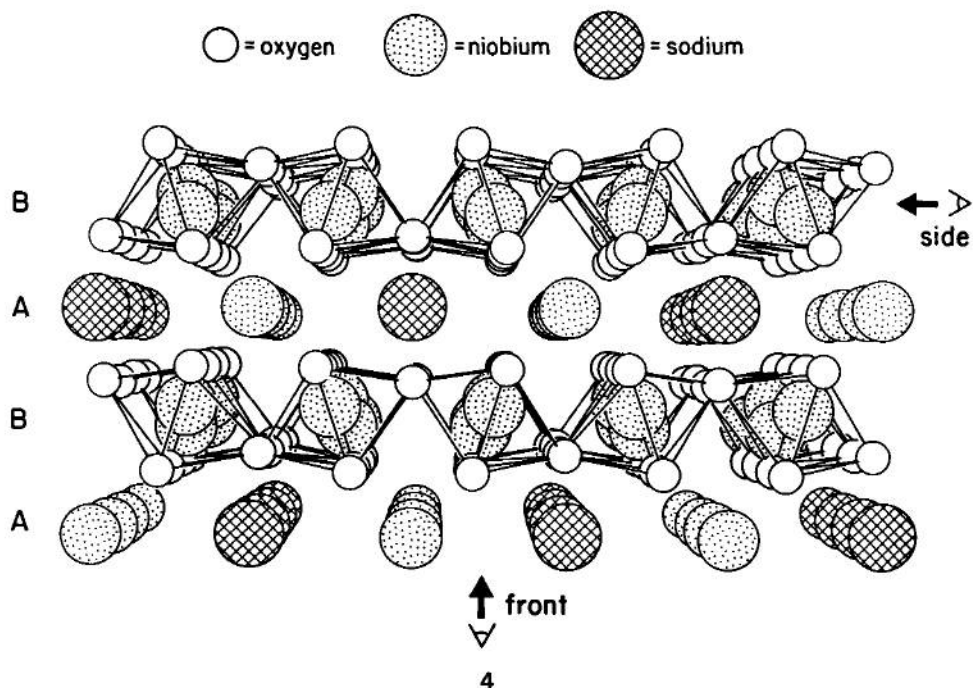
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2



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  $\text{NaNb}_3\text{O}_6$ ,  $\text{NaNb}_3\text{O}_5\text{F}$  and  $\text{Ca}_{0.75}\text{Nb}_3\text{O}_6$ .<sup>7</sup> 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.

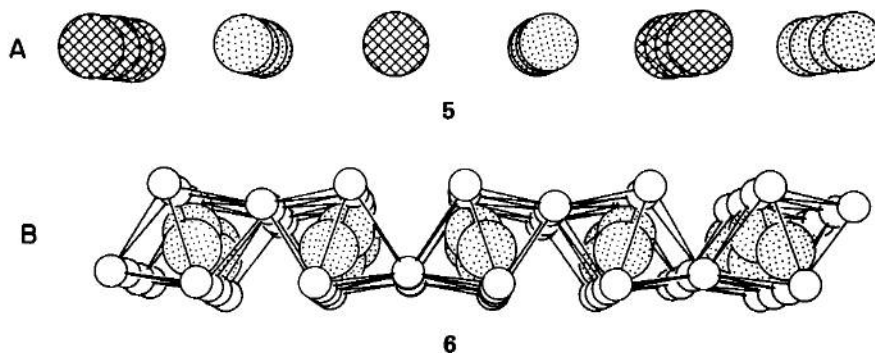
Some conventions: the white balls are oxygens (O), the stippled ones niobium (Nb), the cross-hatched ones sodium (Na). The perspective shown chops out a chunk from the infinite solid, leaving it up to us to extend it, in our mind, in three dimensions. That takes practice.

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

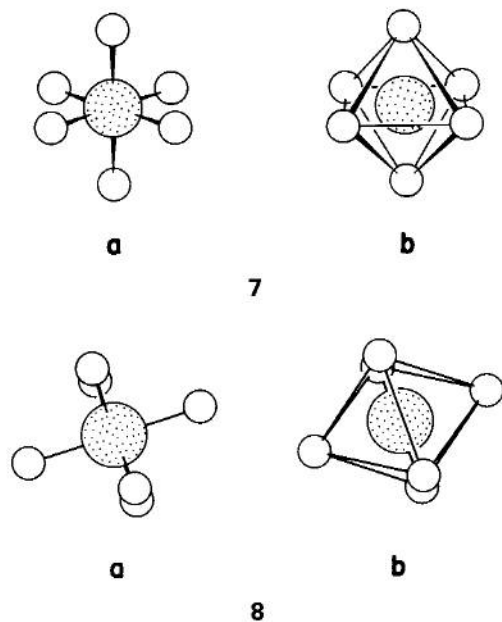
In drawing 4 we clearly see layers or slabs. One layer (marked A) is shown in structure 5. It contains only niobium and sodium atoms. The other layer, B (structure 6), is made up of niobium and oxygen atoms arranged in a seemingly complex kinked lattice-work. Let us take on this B layer first.

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.

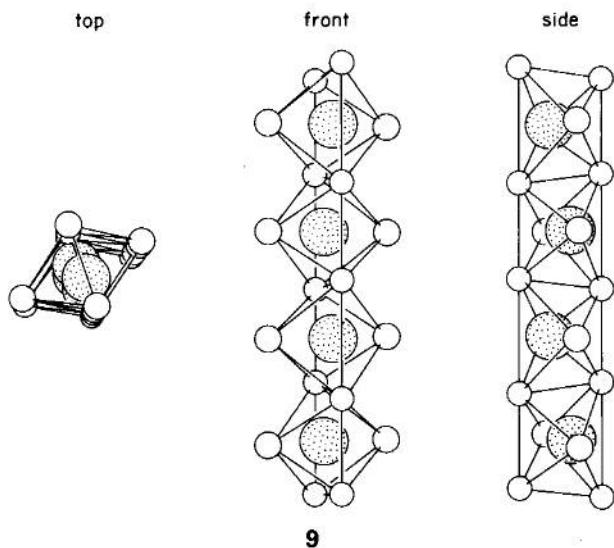
You may wonder where these octahedra are in the



complex structure of  $\text{NaNb}_3\text{O}_6$ . Well, take the octahedra of drawing 7 and rotate them in space, to the viewpoint shown in drawing 8. If you compare 8 with the middle piece of layer B (shown in structure 6), you will see a certain resemblance.



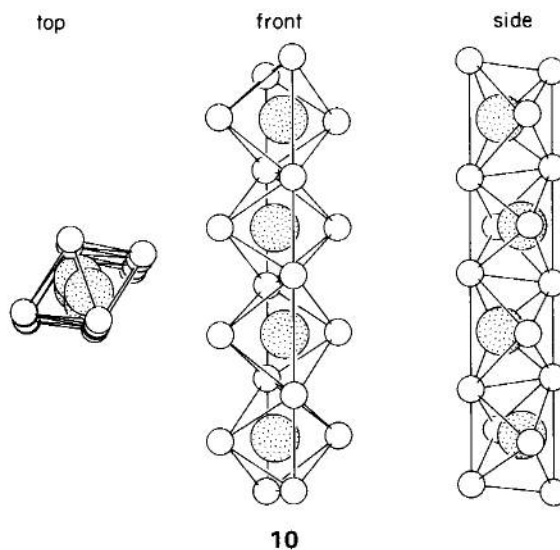
Now consider the structure of the layer. First, a large, semi-infinite number of such octahedra are linked into a one dimensional array by sharing opposite edges. Three views of such an edge sharing octahedral chain are presented in drawing 9.



One of the three views is from the same vantage point as in drawing 4 or 6, say the 'top'. The two other views are roughly from the 'front' and 'side', the viewpoints so marked in the original drawing, 4. The shared edges are emphasised by darker lines in the side view.

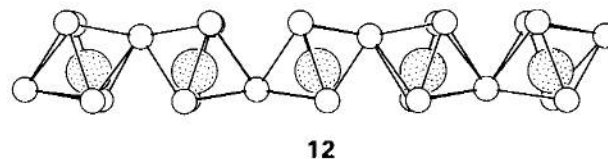
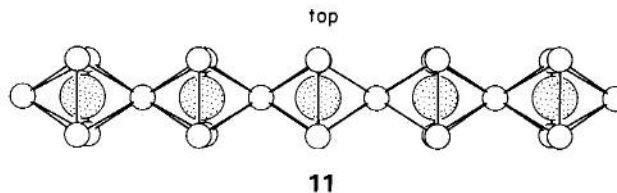
If you compare the top view of one of these infinite chains in drawing 9 with that in 6, you will see a difference – the niobiums are receding from you in a neat straight line in 9, but are 'staggered' in pairs in

6. Indeed, drawing 9 is an idealisation. One of the stacks in the real structure is carved out in drawing 10, shown in the same top view as in 6, but also from the front and the side. The displacement of the niobiums from the centres of the oxygen octahedra, and an associated asymmetry of the oxygens, are clearly visible.



Would you like to know why there occurs this departure from ideality? So did we. A piece of the answer is to be found in a paper that Maria José Calhorda and I have written.<sup>8</sup> For the moment let us accept this symmetrical asymmetry as one of those complexities that makes life interesting.

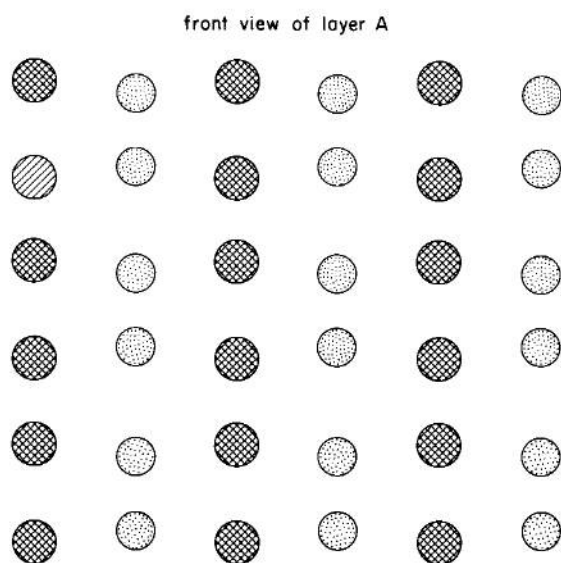
Next, the one dimensional chains of octahedra combine to generate the full B layers by sharing two opposite vertices with identical chains. They could have done so in a nice 'straight' way (*see* drawing 11, a top view of a line of such vertex sharing octahedra). But they do not; they 'kink' (drawing 12) in a less straightforward but still symmetrical way. One gets the feeling that nature is insubordinate... What really is going on, though, is that we, in the weakness of our minds, fix on the first, most symmetrical suggestion of how things might be.



We now have layer B, this fantastic slab (repeated over and over in the crystal) of infinite, one dimensional, edge sharing octahedral chains, in turn stitched

up to a two dimensional slab by sharing vertices. What about layer A?

Drawing 4 shows that layer A is made up of needle-like lines of sodium and niobium. We might think these atoms are equally spaced, but this molecule has another surprise in store for us, as the front view of layer A indicates (drawing 13). Whereas the sodiums are approximately equally spaced, the niobiums clearly are not. They pair along the vertical direction (this pairing is obscured from the 'top' vantage point of drawing 4 or 5), so that there are distinct short (2.6 Å) and long (3.9 Å) Nb-Nb separations. The short one is very short, substantially shorter than that in pure niobium metal.

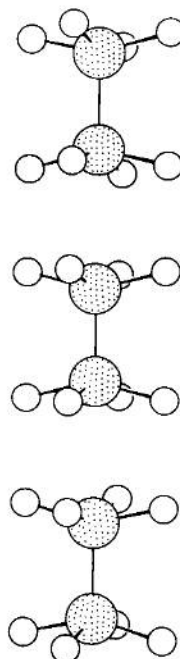


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Why do the niobiums pair? In our study of the way electrons move in these compounds, we find that the pairing is driven by a desire cum necessity to form Nb-Nb bonds along the needle.<sup>8</sup> There are even Nb-Nb bonds, not shown here, between the niobium atoms of stacks A and B.

Other links stitch up the layers. For instance, the niobiums in layer A are not floating in empty space. They are at a bonding distance from the oxygens of two bordering B slabs. In fact, as drawing 14 shows, each pair of niobiums in a line in A nestles comfortably into an array of eight oxygens from layer B. The layers are connected up – this is not a one or two dimensional structure, but a true three dimensional array in which are embedded substructures of lower dimensionality.

Now we have toured the structure, which is at once symmetrical and unsymmetrical, in which the beauty of this aesthetic object resides. The beauty is in the incredible interplay of dimensionality. Think of it: two dimensional slabs are assembled from infinite one dimensional chains of edge sharing octahedra of oxygens around niobium, which in turn share vertices. These two dimensional slabs interlink to the full three dimensional structure by bonding with one dimen-



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sional needles of niobium and sodium. And then, in a final twist of the molecular scenario, these one dimensional needles pair up niobiums, declining to space equally. The  $\text{NaNb}_3\text{O}_6$  structure selfassembles, in small black crystals, an aesthetic testimonial to the natural forces that shape the molecule, and to the beauty of the human mind and hands that unnaturally brought this structure into being.

## Kant

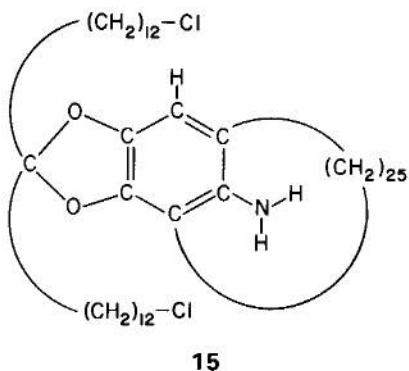
It is hard to escape the feeling that a chemist appreciative of the dimensional ins and outs of  $\text{NaNb}_3\text{O}_6$  is doing just what Kant described in the following words:

He who feels pleasure in the mere reflection upon the form of an object...justly claims the agreement of all men, because the ground of this pleasure is found in the universal, although subjective, condition of reflective judgments, viz. the purposive harmony of an object (whether a product of nature or of art) with the mutual relations of the cognitive faculties (the imagination and the understanding)...<sup>9</sup>

But let us go on, to look at another source of molecular beauty.

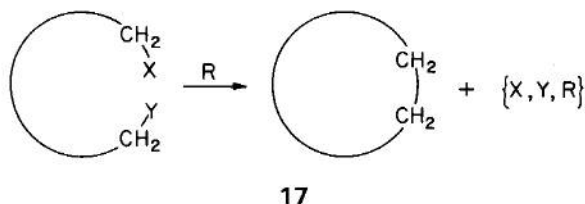
## Frogs about to be kissed

Could one say much by way of approbation for molecule 15? Not at first sight. What are those dangling  $(\text{CH})_{12}\text{-Cl}$  chains on the left? Or the unsymmetrical  $(\text{CH}_2)_{25}$  loop on the right, or the  $\text{NH}_2$  group? The molecule is, if not ugly (there are no ugly molecules, says this most prejudiced chemist), at least plain. It's not an essential component of life, it's not produced in gigakilogram lots. In fact its purpose in life is not clear.



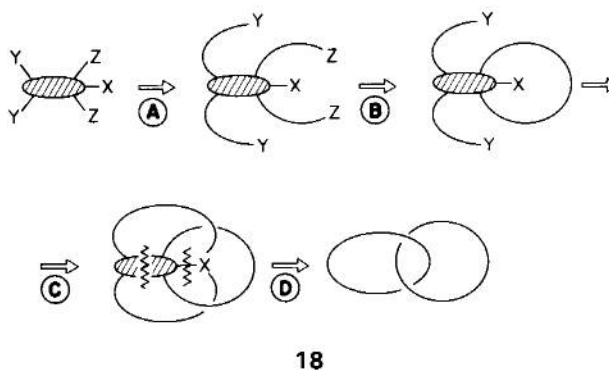
The last sentence contains a clue to what makes this molecule, a frog that is a prince, beautiful. Chemistry is molecules, and it is chemical change, the transformations of molecules. Beauty or elegance may reside, static, in the very structure, as we saw for the molecule  $\text{NaNb}_3\text{O}_6$ . Or it may be found in the process of moving from where one was to where one wants to be. Historicity and intent have incredible transforming power; this molecule is beautiful because it is a waypoint. Or as they say in the trade, an intermediate.

So: *quo vadis?* To a catenane, structure 16, two interlocking rings of carbon atoms, not chemically combined but held together like the links of a chain. Why should people try to make a catenane? For no particular reason. For the best reason, because none was made before. How to make it? Here is one strategy, which I will term a statistical one. A typical chemical reaction is a cyclisation, schematically written out in structure 17. If we run the cyclisation of a long chain, some fraction of the time – purely by chance – the chains will be entwined, or a chain will be threaded through an already formed ring, in such a way that a catenane will be formed. Remember how small molecules are, how many ( $10^{20}$ ) there are in a typical pot. In all this multitude, statistics have a chance to work. E. Wasserman actually realised this in 1960, synthesising a catenane<sup>10</sup> for the first time.



The statistical procedure works, albeit inefficiently. There are other ways to craft the catenane topology. One beautifully conceived synthesis is due to Schill and Lüttringhaus.<sup>11</sup> Their logical scheme is summarised in chart 18. The starting point is a molecule with lots of specifically disposed functionality. In chemis-

try, a functional group is a set of bonded atoms whose properties are more or less invariant from one molecule to another. The most important of these properties is chemical reactivity, the 'function' of the group. To put it another way, in the context of doing chemistry on a molecule, functional groups are the *handles* on a molecule. The transformations of functional groups, and particularly the predictability of their reactions, are a crucial element in the conceptual design of syntheses in organic chemistry. Common functional groups might be  $\text{R-OH}$  (alcohols),  $\text{R-COOH}$  (organic acids),  $\text{R-COH}$  (aldehydes) or  $\text{R-X}$  ( $\text{X}=\text{F}, \text{Cl}, \text{Br}, \text{I}$ : the halides), where  $\text{R}$  is anything. The substituents  $\text{X}, \text{Y}$  and  $\text{Z}$  in structure 18 are functional groups.

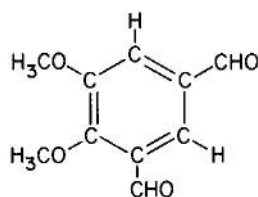


Step A in structure 18 elaborates the  $\text{Y}$  and  $\text{Z}$  functional group handles into long chains. Step B is a closing up, or 'cyclisation', of one set of chains. Step C is a different kind of cyclisation, another linking up, now of the other set of chains to the remaining core functionality  $\text{X}$ . Step D, perhaps several steps, is a fragmentation, in which the core from which the reaction was initiated, on which all was built, is now mercilessly torn apart, revealing the catenane.

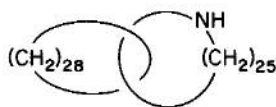
Several points about this process are important: (i) the synthesis is architecture, a building, and (ii) as such it requires work. It is easy to write down the logical sequence of steps as I have. But each step may be several chemical reactions, and each reaction a more or less elaborate set of physical processes. These take time and money; (iii) the architectonic nature of the process almost dictates that the middle of the construction is characterised by molecules that are more complex than those at the beginning and the end.<sup>12</sup> Note (iv) the essential topological context of chemistry. It is evident not only in the curious topology of the goal, a catenane, but also in the very process of linkage that pervades this magnificent way of building.

To return to the reality of the specific, the moment scheme 18 is laid out it is clear what molecule 15 is. It is the crucial point in the middle, after step B, before step C. It is poised to cyclise, the chlorines at the end of the  $(\text{CH}_2)_{12}$  chains set to react with the  $\text{NH}_2$  group. The synthesis by Schill and Lüttringhaus begins with molecule 19 and ends with catenane 20,

in which a ring of 28 carbons interlocks with another ring with 25 carbons and one nitrogen. But while getting to structure 20 is sweet, it should be clear that what is important is *getting to*, the process. That process is reasonably linear (although chart 18 makes us think it is more linear than it is). One might suppose that any step in a linear chain of transformations ( $a \rightarrow b \rightarrow c \rightarrow d \rightarrow e$ ) could claim primacy of significance. Indeed the steps in a synthesis may differ vastly in their difficulty, and therefore in the ingenuity invested to accomplish them. The unpublished lore of chemistry abounds with tales of a fantastically conceived, elegant synthesis in which the very last step, thought to be trivial, fails.

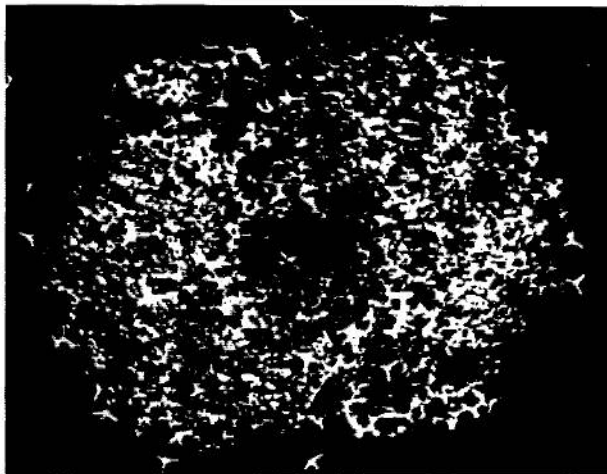


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tight complexity. It looks like a clump of pasta congealed from primordial soup or a tapeworm quadrille. The molecule's shape and function are enigmatic (until we know what it is!). It is not beautifully simple.



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Nevertheless, I will advocate a special claim for a molecule somewhere in the middle of the scheme, the molecule most complicated relative to the starting materials and the goal; the molecule most disguised, yet the one bearing in it, obvious to its conceiver but to few others, the surprise, the essence of what is to come.<sup>13</sup> It is the col of complexity, and the only way from this beautiful molecule is on, on.

## A position on utility

The last section, if it correctly describes a prevalent feature of beauty in the mind of the chemist (and I assure you it does), departs substantially from a Kantian perspective.<sup>14</sup> There is *Zweckmässigkeit* [purposive intent] in abundance in molecule 15, but it is powered by *Zweck* [purpose], the catenane.

Detachment has been central in analytic theories of aesthetics. Some frameworks have introduced a stronger quality, disinterest. To Kant an object that is of utility (for instance, the catenane precursor, not to speak of an antibiotic or sulphuric acid, made in a mere 110 million tonnes worldwide this year), whose valuation is not sensually immediate but requires cognitive action, cannot qualify as being beautiful. As several commentators have pointed out, this is a rather impoverishing restriction on our aesthetic judgments.<sup>15,16</sup> It seems clear to me that knowledge – of origins, causes, relations and utility – enhances pleasure. Perhaps that cognitive enhancement is greater in scientific perusal, but I would claim that it applies as well to a poem by Ezra Pound.

But let us go on.

## As rich as need be

Look at molecule 21. It seems there's nothing beautiful in its involuted curves, no apparent order in its

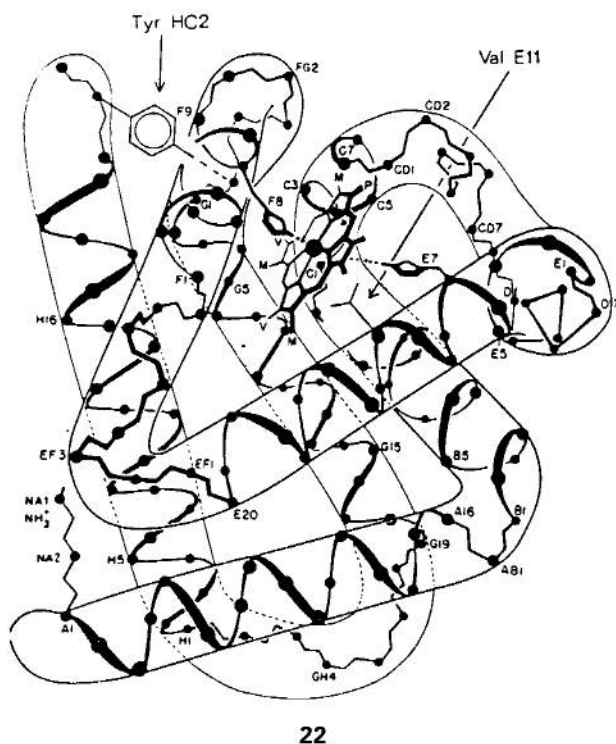
Complexity poses problems in any aesthetic, that of the visual arts and music as well as chemistry. There are times when the *Zeitgeist* seems to crave fussy detail – Victorian times, the rococo. Such periods alternate with ones in which the plain is valued. Deep down, the complex and the simple coexist and reinforce each other. Thus the classic purity of a Greek temple was set off by sculptural friezes, the pediments and the statues inside. The clean lines and functional simplicity of Bauhaus or Scandinavian furniture owe much to the clever complexity of the materials and the way they are joined. Elliott Carter's musical compositions may seem difficult to listen to, but their separate instrumental parts follow a clear line.

In science, simplicity and complexity always coexist. The world of real phenomena is intricate, the underlying principles simpler, if not as simple as our naive minds imagine them to be. But perhaps chemistry, the central science, *is* different, for in it complexity is central. I call it simply richness, the realm of the possible.

Chemistry is the science of molecules and their transformations. It is the science not so much of the hundred elements, but of the infinite variety of molecules that may be built from them. You want it simple – a molecule shaped like a tetrahedron or the cubic lattice of rock salt? We have got it for you. You want it complex – intricate enough to run efficiently a body with its 10 000 concurrent chemical reactions? We have that too. Do you want it done differently – a male hormone here, a female hormone there; the blue of cornflowers or the red of a poppy? No problem, a mere change of a  $\text{CH}_3$  group or a proton respectively will tune it. A few million generations of evolutionary tinkering, a few months in a glass glittery lab, and it is done! Chemists (and nature)

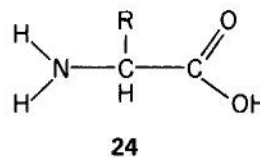
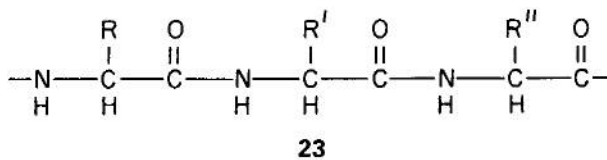
make molecules in all their splendiferous functional complexity.

Beautiful molecule 21 is haemoglobin, the oxygen transport protein. Like many proteins, it is assembled from several fitted chunks, or subunits. The subunits come in two pairs, called  $\alpha$  and  $\beta$ . Incredibly, these actually change chemically twice in the course of foetal development, so as to optimise oxygen uptake. The way the four subunits of haemoglobin mesh, their interface, is requisite for the protein's task, which is to take oxygen from the lungs to the cells.<sup>17</sup>



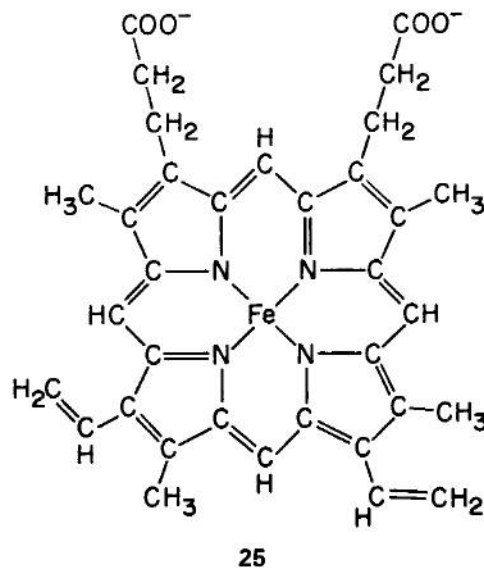
One of the haemoglobin subunits is shown in structure 22. It is a curled up polypeptide chain carrying a 'haeme' molecule nestled within the curves of the chain. All proteins, not just haemoglobin, contain such polypeptide chains (see structure 23 for a schematic formula), which are assembled in turn by condensation of the building block amino acids, shown in structure 24. These come in about 20 varieties, distinguished by their 'side chains' (R in structures 23 and 24). A typical protein, the haemoglobin  $\beta$  chain is made up of 146 amino acid links. Here is riches, reaching out to us! Think how many 146 link chain molecules there could be given the freedom to choose the side chains in 20 possible ways. The incredible range of chemical structure and function that we see in those tiny molecular factories, enzymes, or in other proteins, derives from that variety. The side chains are not adornment, they make for function.

The protein folds, the diversity of the side chains provides opportunity, the particular amino acid sequence enforces a specific geometry and function. Extended pieces of haemoglobin curl in helical sections, clearly visible in structure 22. At other places



the chain kinks, not at random, but preferentially at one amino acid, called proline. The globular tumble of helical sections, nothing simple, but functionally significant, emerges.

Significant in what way? To *hold* the molecular piece that binds the oxygen, and to *change*, in a certain way, once the oxygen is bound. The O<sub>2</sub> winds its way into a pocket in the protein that is just right, and binds to the flat, disc shaped haeme molecule. The structure of haeme is shown in 25. The oxygen binds, end on, to the iron at the centre of the haeme. As it does, the iron changes its position a little, the haeme flexes, the surrounding protein moves. In a cascade of well engineered molecular motions the oxygenation of one subunit is communicated to another, rendering that one more susceptible to taking up another O<sub>2</sub> molecule.



That bizarre sculpted folding has a purpose, in the structure and function of a molecule critical to life. All of a sudden we see it in its dazzling beauty. So much so that it cries out 'I've been designed'; 'For this task, I'm the best that can be'. Or, if you are so inclined, it testifies to a Designer.

Beautiful? Certainly. The best, fashioned to a plan? Hardly. It only takes a moment to get us back to Earth, a few bubbles of CO, the lethal, odourless product of incomplete combustion of fires and car exhausts. Carbon monoxide fits into the same wondrously designed protein pocket, and it binds to

haemoglobin several hundred times better than oxygen.

So much for the best of all possible worlds and the evolutionary plan. As F. Jacob has written, nature is a tinkerer.<sup>18</sup> It has a wonderful mechanism for exploring chance variation, and, until we came along, much time on its hands. While it was banging haemoglobin into shape there was not much carbon monoxide around. So it never 'worried' about it.

Actually the story, the story of molecular evolution, is more complicated, more wondrous still. It turns out that there is always a bit of carbon monoxide around in the body, a natural product of cellular processes. Haeme, free of its protein, binds carbon monoxide much better than haemoglobin. So the protein around the haeme apparently evolved to *discourage* carbon monoxide bonding a little. Not enough to take care of massive doses of external carbon monoxide, just enough to allow the protein to take up sufficient oxygen even in the presence of naturally produced carbon monoxide.<sup>17</sup>

## Iconicity

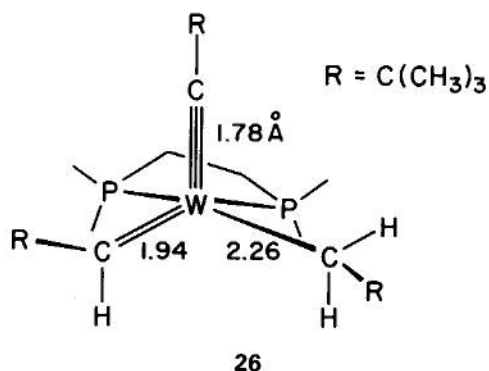
A word might be in place here about the preponderance of visual representations of molecules in this exposition. Could I be overemphasising the *picture* of the molecule in analysing the pleasure chemists take, at the expense of the *reality* of molecules and their transformations?

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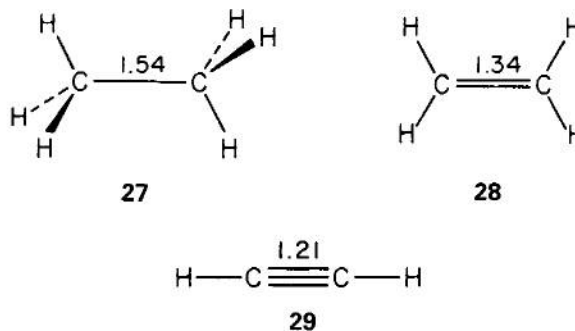
## Archetypes and epitomes

Classical notions of beauty do have a hold on us. Central to Plato's and Aristotle's notions of reality was the ideal of a universal form or essence. Real objects are an approximation to that form. Art, in dismissive moments, was to the Greek philosophers mere imitation or, more positively, something akin to science, a search for the essential core. Concepts such as the archetype and the epitome figure in the Greek aesthetic. And they are to be found in chemistry today. The archetype is the ideal simple parent molecule of a group of derivatives, say methane (CH<sub>4</sub>), and not any of the myriad substituted methanes CRR'R''R''' which make life interesting.

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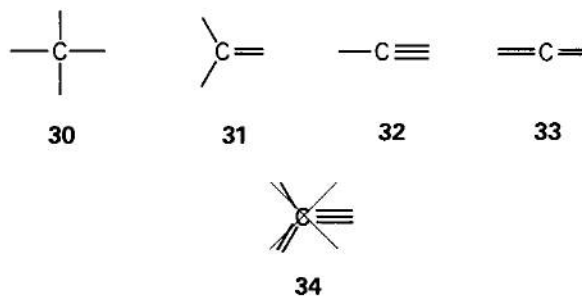


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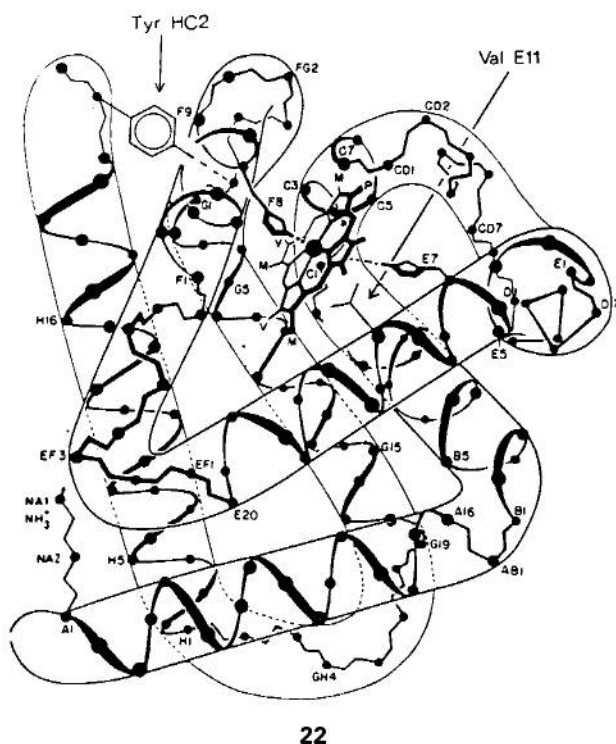
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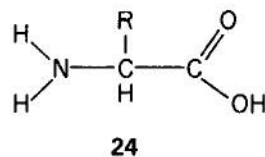
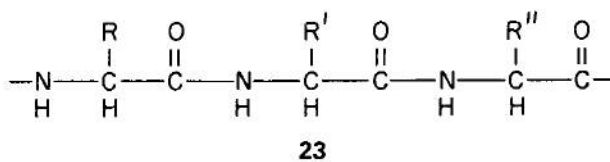
make molecules in all their splendiferous functional complexity.

Beautiful molecule 21 is haemoglobin, the oxygen transport protein. Like many proteins, it is assembled from several fitted chunks, or subunits. The subunits come in two pairs, called  $\alpha$  and  $\beta$ . Incredibly, these actually change chemically twice in the course of foetal development, so as to optimise oxygen uptake. The way the four subunits of haemoglobin mesh, their interface, is requisite for the protein's task, which is to take oxygen from the lungs to the cells.<sup>17</sup>



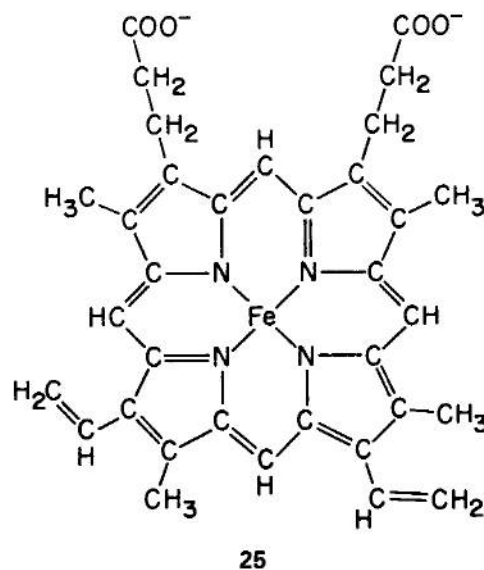
One of the haemoglobin subunits is shown in structure 22. It is a curled up polypeptide chain carrying a 'haeme' molecule nestled within the curves of the chain. All proteins, not just haemoglobin, contain such polypeptide chains (see structure 23 for a schematic formula), which are assembled in turn by condensation of the building block amino acids, shown in structure 24. These come in about 20 varieties, distinguished by their 'side chains' (R in structures 23 and 24). A typical protein, the haemoglobin  $\beta$  chain is made up of 146 amino acid links. Here is riches, reaching out to us! Think how many 146 link chain molecules there could be given the freedom to choose the side chains in 20 possible ways. The incredible range of chemical structure and function that we see in those tiny molecular factories, enzymes, or in other proteins, derives from that variety. The side chains are not adornment, they make for function.

The protein folds, the diversity of the side chains provides opportunity, the particular amino acid sequence enforces a specific geometry and function. Extended pieces of haemoglobin curl in helical sections, clearly visible in structure 22. At other places



the chain kinks, not at random, but preferentially at one amino acid, called proline. The globular tumble of helical sections, nothing simple, but functionally significant, emerges.

Significant in what way? To hold the molecular piece that binds the oxygen, and to change, in a certain way, once the oxygen is bound. The  $O_2$  winds its way into a pocket in the protein that is just right, and binds to the flat, disc shaped haeme molecule. The structure of haeme is shown in 25. The oxygen binds, end on, to the iron at the centre of the haeme. As it does, the iron changes its position a little, the haeme flexes, the surrounding protein moves. In a cascade of well engineered molecular motions the oxygenation of one subunit is communicated to another, rendering that one more susceptible to taking up another  $O_2$  molecule.



That bizarre sculpted folding has a purpose, in the structure and function of a molecule critical to life. All of a sudden we see it in its dazzling beauty. So much so that it cries out 'I've been designed'; 'For this task, I'm the best that can be'. Or, if you are so inclined, it testifies to a Designer.

Beautiful? Certainly. The best, fashioned to a plan? Hardly. It only takes a moment to get us back to Earth, a few bubbles of CO, the lethal, odourless product of incomplete combustion of fires and car exhausts. Carbon monoxide fits into the same wondrously designed protein pocket, and it binds to

haemoglobin several hundred times better than oxygen.

So much for the best of all possible worlds and the evolutionary plan. As F. Jacob has written, nature is a tinkerer.<sup>18</sup> It has a wonderful mechanism for exploring chance variation, and, until we came along, much time on its hands. While it was banging haemoglobin into shape there was not much carbon monoxide around. So it never 'worried' about it.

Actually the story, the story of molecular evolution, is more complicated, more wondrous still. It turns out that there is always a bit of carbon monoxide around in the body, a natural product of cellular processes. Haeme, free of its protein, binds carbon monoxide much better than haemoglobin. So the protein around the haeme apparently evolved to *discourage* carbon monoxide bonding a little. Not enough to take care of massive doses of external carbon monoxide, just enough to allow the protein to take up sufficient oxygen even in the presence of naturally produced carbon monoxide.<sup>17</sup>

## Iconicity

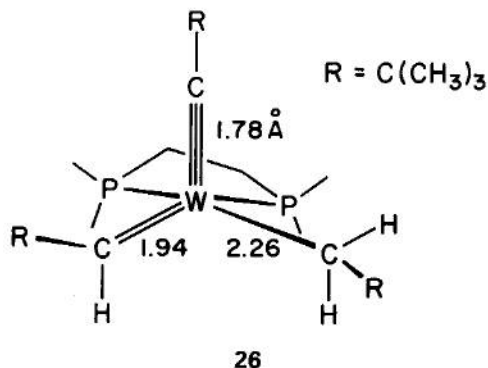
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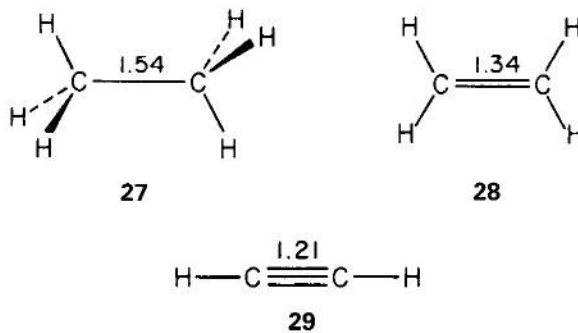
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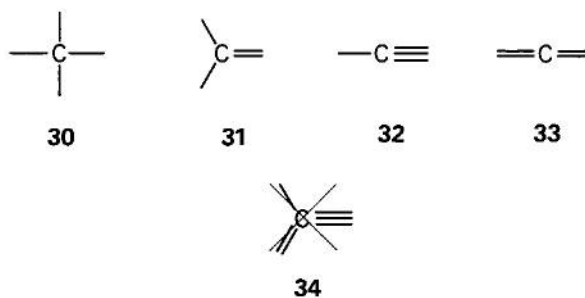


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only four bonds, you cannot have molecule 34, a carbon atom with a single, double and triple bond to it.

Not so for metals. The 'transition metals' – chromium, iron, manganese, cobalt, nickel, rhenium, tungsten and so on – have the capacity to form up to nine bonds. The chemistry of metal to other element bonds, especially the metal–carbon single bond, is nearly 40 years young, that of metal–carbon double and triple bonds younger still. This is the burgeoning realm of organometallic chemistry. The concentrated beauty of structure 26 lies in that it is a molecule in which one and the same tungsten atom forms a single W–C bond, a double one and a triple one. And two bonds to phosphorus, for good measure. Incidentally structure 26's official name is [1,2bis(dimethylphosphino)ethane](neopentylidyne)(neopentylidene)(neopentyl)tungsten(VI)!

Such bonds are present, individually, in many molecules made in the past four decades. But in structure 26 they are all in one. The epitome, for that is what molecule 26 is, intensifies what it exemplifies by concentrating several disjoint examples into one. Its psychological impact is more than the sum of its parts; by such concentration it enhances our aesthetic response.

## Novelty

Note the strong intrusion of the cognitive into judgments of the beauty of the molecules in the previous section. Their beauty is dependent, to use the Kantian term, they are very special members of a class. Still more dependent, in fact stretching outside of the limits of what is usually considered a viable aesthetic quality, is what characterises the molecules of this section. It is *novelty*. I would claim that in the minds of chemists the new can leap the gap between 'interesting' and 'beautiful'.

Science certainly subscribes in its very structure to the idea of innovation. It may be discovery – understanding how haemoglobin, discussed above, works. Or finding out how pre-Colombian Andean metal-

smiths electroplated gold without electricity.<sup>21</sup> It may be creation – the synthesis of the catenane 16, or the tungsten compound 26.

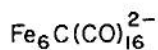
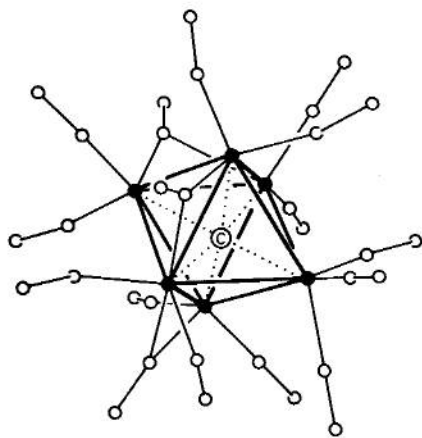
We are addicted to new knowledge, and we value it (therefore it is interesting to reflect on the generally conservative tastes of scientists in art, or their astonishment that some other people do not view scientific or technological innovation as an absolute good). At the same time most chemistry builds slowly. It is paradigmatic science, routine if not hack work, extending step by patient step what has been done before. Chemists appreciate this patient work, it allows them to read a new issue of a journal quickly. Yet it is inevitable that they grow just a bit bored by its steady drone, its familiar harmony.

Then, all of a sudden, from the plain of fumaroles, an eruption of fire reaches for the sky. It is impossible not to look at it, it is a hot intrusion on the landscape of the mind, as beautiful as it is new. A surprising, unexpected molecule.

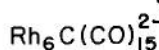
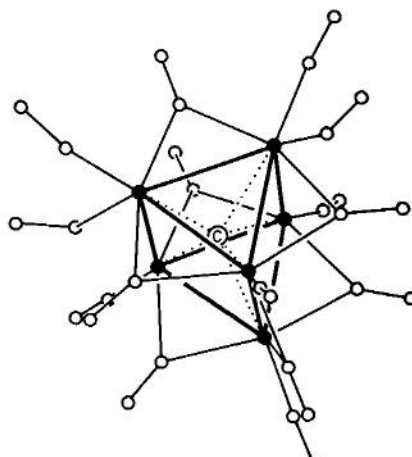
Two examples come to mind, in counterpoint to the organometallic epitome. The long accepted inability of carbon to form more than four bonds is the fertile ground from which grow millions of natural and synthetic products, all the beauty of life and the democratising utility of modern chemistry. But it is not holy ground, this four coordination of carbon.

Some time ago, inorganic chemists made molecules 35 and 36, called metal carbonyl clusters.<sup>22</sup> In these the metal atoms form a lovely symmetrical polyhedron – an octahedron of irons in structure 35, a trigonal prism of rhodiums in 36. Around that polyhedron, seemingly loosely scattered on its periphery, are carbon monoxides, called carbonyls. And in the centre, captive, encapsulated, resides a single carbon atom. It is connected to, equidistant from, all six metals around it.

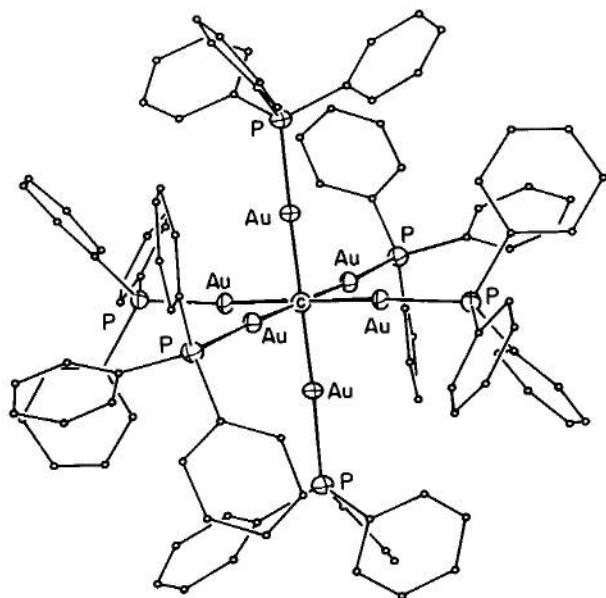
More recently, Schmidbaur and co-workers in Munich<sup>23</sup> made a not unrelated, spectacularly simple molecule, 37. In it, central, is a lone carbon. Bonded radially to it are six ligands, AuPR<sub>3</sub> groups. There is a plus two charge on this molecule.



35



36



37

In these compounds (molecules 35–37) carbon patently forms six bonds. This is the surprise, the shock, the full impact of which should (but has not yet) hit every maker of carbon compounds.<sup>24</sup> It makes these metal carbonyl clusters and the  $C(AuPR_3)_6^{2+}$  molecule beautiful. They are new, interesting and lovely.

And they pose questions. How can carbon form six bonds? Are the old ideas wrong? Not entirely, for when we look at how the electrons move in these molecules we find that these are different kinds of bonds, perhaps weaker individually than normal carbon's four classical bonds. Theory expands to accommodate the new; the novel in time will become routine, only to be shaken by the unforeseen violator of the new set of rules.

## Empirical chemical aesthetics and formal theories

I have hardly exhausted the capacity of molecular creation to please the human mind. Molecules can be beautiful because of the wondrous quantised motions they undergo, truly a music played out in tones, harmonics and overtones that our instruments, now measuring instruments, hear. They may be beautified by their miracles – who would deny it to penicillin or morphine? Or more lowly, they may be as beautiful as the 5 million tonnes of phosphoric acid ( $H_3PO_4$ ) manufactured every year. You are more likely to have heard of the rougher guys, the spectacular hydrochloric, nitric and sulphuric siblings. But this quiet one is responsible for a good part of the essential phosphorus in your DNA.

Much philosophic tradition would object to including the utilitarian perspective as an aesthetic criterion. I have mentioned above some objection to this limiting view. Here I would only add the empirical testimony of the practitioners – be they deluded, naive or not, chemists really do think that *use* is an element,

not the most important one, but an element of chemical beauty.

But perhaps it is time to stop here and take another tack. Let us posit that we have discovered in this anthropological study of chemistry a reliable sampling of the qualities the experts/natives use as attributes of beauty. They, the chemists, we, for I am among them, have an aesthetic. Maybe we do not call any molecule ugly, but some molecules are more beautiful than others. Does our aesthetic, our way of assigning beauty, have something in common with the aesthetics characteristic of other parts of human experience, those of games, of business, of love, but especially of art?

I am not going to answer this question here to anyone's satisfaction, but it is worth asking. A fundamental problem, of course, is that aesthetics is not a closed chapter of philosophy. Rival theories abound, indeed the dialogue shifts with time, much as the subject of its discussion. Nevertheless, one could proceed by seeing how the concept of beauty in chemistry fits or does not fit into the existing (fashionable?) aesthetic frameworks erected by philosophers. This has been done to some extent in the sections above, but let me approach the problem more directly here.

For instance, Monroe Beardsley supposes that the aesthetic response (to a work of art, which is an artifact intended to elicit such a response) entails importantly a degree of detachment on the part of the viewer or listener and the elements of intensity, unity and complexity in the object viewed.<sup>25</sup> His argument deserves deeper exposition than these few words, but it seems to me that the chemist's aesthetic response entails many of Beardsley's factors. As for detachment, a concentration that envelops, well – the only people I have seen more detached than chemists looking at molecules are computer hackers or Pachinko players. Intensity has been discussed in the previous section, in the context of molecule 26. It said a lot, economically. Unity is by and large absent in the exemplars selected by me. They stand alone. But, implicitly, these structures cannot be viewed as beautiful except in the context of knowledge of other molecules. And if they be totally new, they impose a stress on existing theories to assimilate their brash flaunting of not fitting in. New molecules incite theory, which is the unifying, framework building way the chemist makes connections.

I hesitate on complexity, not because it is unimportant (remember haemoglobin and all your enzymes) but because I see so clearly the aesthetic strength of simplicity. The parent molecule, the symmetrical molecule, the reaction that goes under wide conditions, the simple mechanism, the underlying theory expressed by a single mathematical equation – these have beauty conferring value.

However, there is a thread that runs through the tokens of chemical beauty that inclines me to another aesthetic philosophy, which is that of Nelson Goodman.<sup>26</sup> Goodman views science and art both as

cognitive processes, differing perhaps only in their intensity or degree of elaboration or manipulation of symbols. And one is certainly struck by the cognitive element in all these appreciations of the chemist, in our reactions to molecules. We feel that these molecules are beautiful, that they express essences. We feel it emotionally, let no one doubt that. But the main predisposition that allows the emotion, here psychological satisfaction, to act, is one of knowing, of seeing relationships. I took apart  $\text{NaNb}_3\text{O}_6$  into chains of octahedra and layers, and related it so to other materials. I saw the catenane synthesis planned, and so grew to love the molecule at its high pass. I know what haemoglobin does, therefore I care about it. And the molecules in the preceding section are clearly fascinating because they stand out, or soar.

Perhaps we should not press too hard to fit the multifarious manifestations of chemical beauty into tight categories or theoretical frameworks. Even if we were to agree on a definition of beauty, what would it gain us? As M. H. Abrams has pointed out,<sup>27</sup> saying that X is beautiful is almost the dullest thing one can say about X. One needs to describe the object's attractiveness. I hope that this essay has done so, part way, for molecules.<sup>28</sup>

These products of our hands and minds, beautiful molecules, appeal directly to the mind. For a chemist, their line into the soul is direct, empowering, sometimes searing. They are natural, haemoglobin like a fern unfurling, like the cry of a duck on a winter lake. They are synthetic (or if you like artifactual, man or woman made, unnatural) – the catenane, Schrock's tungsten epitome, like the Shaker tune "tis a gift to be simple", like Ogata Korin's screens.

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  26. N. GOODMAN: 'Languages of art', 2nd edn; 1976, Indianapolis, IN, Hackett Publishing Co.
  27. M. H. ABRAMS: personal communication. See also G. SIRCELLO: 'A new theory of beauty', 118–121; 1975, Princeton, NJ, Princeton University Press.
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