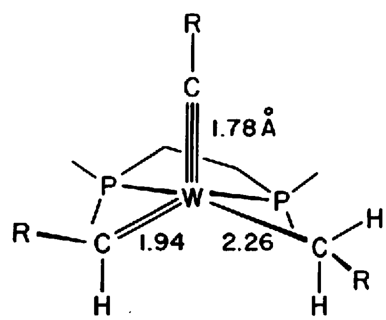
Marginalia

Molecular Beauty IV: Toward an Aesthetic Theory of Six-coordinate Carbon

Roald Hoffmann

Classical notions of beauty still have a hold on us. For Plato and Aristotle, central to the notion of reality was the ideal of a universal form or essence. Real objects were considered an approximation to that form. Art was to the Greek philosophers (in dismissive moments) 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_4, and not any of the myriad substituted methanes such as CRR′R″R‴, which make life interesting.



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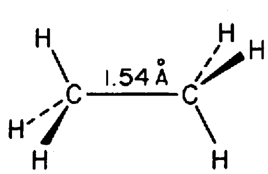
The epitome is something typical, but possessing the features of a class to a high degree. It is this concentration of feeling which I want to focus on, for it is one of the determinants of beauty in chemistry. Molecule 1 (synthesis by Clark and Schrock, structure determined by Churchill and Youngs, *1)* is such an emblem, but we must set the background in order for its compressed beauty to emerge.

Molecules exist because there are bonds, the electronic glue that binds atoms together. In organic chemistry, bonds come in several types—single as in ethane (structure 2), double as in ethylene (structure 3), triple as in acetylene (structure 4). The plain English words tell the story: double is stronger than single, and triple is stronger still. The length of the bonds correlates with their strength, for chemical bonds act much like springs. Thus the atoms held together by a triple bond are more tightly bound and the bond between them is shorter in length than a double bond; the latter in turn is shorter than a single bond.



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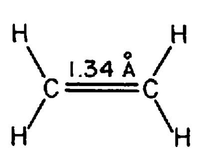

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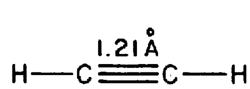

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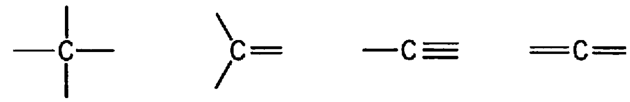
You can mix bond types—that is, make four single bonds to a carbon, or two single ones and a double, or a single and a triple, or two double bonds (structure 5). But because carbon has the capability of forming—in general (more on this later)—only four bonds, you cannot have molecule 6, a carbon atom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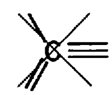
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with a single, double, and triple bond to it.

Not so for metals. The "transition metals"—chromium, iron, manganese, cobalt, nickel, rhenium, tungsten, etc.—have the capacity to form up to nine bonds. The chemistry of bonds between metals and other elements, especially the metal-carbon single bond, is nearly 40 years young; that of metal-carbon double and triple bonds is younger still. This is the burgeoning realm of organometallic chemistry. Structure 1 exhibits the concentrated beauty of a molecule in which one and the same tungsten atom forms a single tungsten-carbon bond, a double one, and a triple one. And two bonds to phosphorus, for good measure.

Such bonds are present, individually, in many molecules made in the last four decades. But in structure 1 they're all in one place *(1)*. The epitome, for that is what molecule 1 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 compression it enhances our aesthetic response.

The contrast of the organometallic epitome to the background of normal bonding in organic chemistry—the chemistry of carbon—brings us to another signature of molecular beauty, which is novelty.

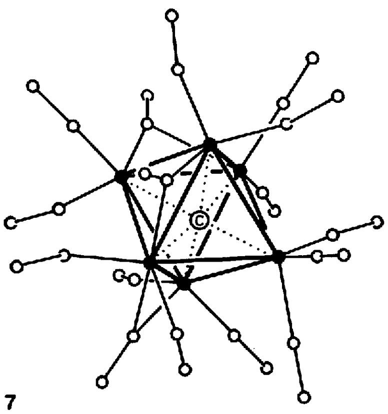
Science subscribes in its very structure to the idea of innovation. It may be discovery—understanding how hemoglobin, the subject of my preceding Marginalium, works. Or finding out how pre-Columbian Andean metalsmiths electroplated gold without electricity *(2)*. It may be creation—the synthesis of the catenane of two Marginalia ago, or the tungsten compound of structure 1.

We are addicted to new knowledge, and we value it. (Therefore it's interesting to reflect on the generally conservative tastes of scientists in art, or their astonishment that some other people don't 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 normal 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, a geyser of fire reaches for the sky. It's 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 volcanic ground from which grow millions of natural and synthetic products, all the beauty of life, and the democratizing utility of modern chemistry. But it is not holy ground, this four-coordination of carbon.

Some time ago, inorganic chemists made molecules 7 and 8, called metal carbonyl clusters *(3)*. In these the metal atoms form a lovely symmetrical polyhedron—an



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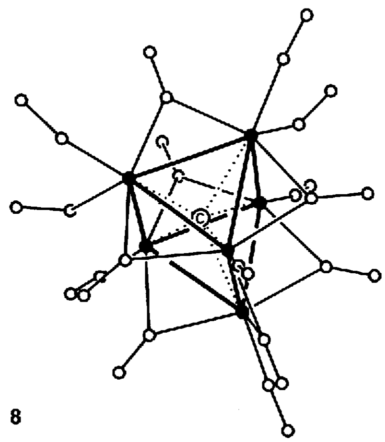

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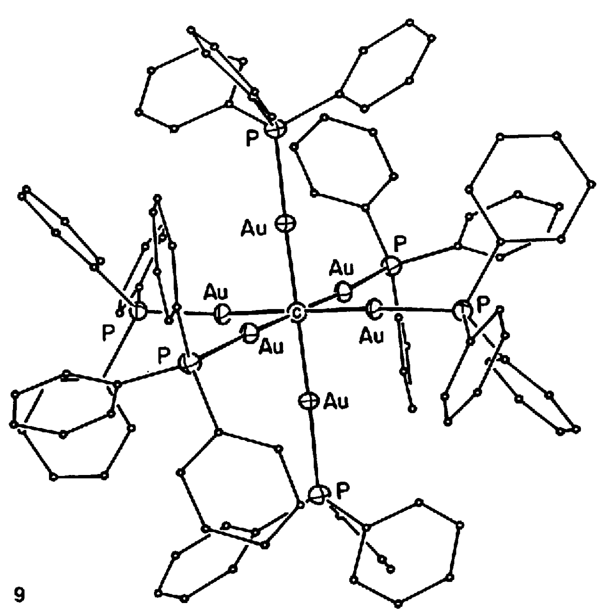
octahedron of irons in structure 7, a trigonal prism of rhodiums in 8. Around that polyhedron, seemingly loosely scattered on its periphery, are carbon monoxides, called carbonyls. And in the center, captive, encapsulated, resides a single carbon atom. It is connected to and equidistant from all *six* metals around it.

More recently, in fact just a few months ago, H.



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Schmidbaur and his co-workers in Munich *(4)* made a not-unrelated, spectacularly simple molecule, 9. In it, central, is a lone carbon. Bonded radially to it are six ligands, $AuPR_3$ groups. There is a charge of +2 on this molecule.

In these compounds (molecules 7, 8, and 9) carbon patently forms six bonds. This is the surprise, the shock—the full impact of which should (but hasn't yet) hit every maker of carbon compounds *(5)*. 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.

This is the fourth Marginalium on the chemist's aesthetic, but I have hardly exhausted the capacity of molecular creation to please the human mind. Molecules can be beautiful because of the wondrous quantized motions they undergo, truly a music played out in tones, harmonics, and overtones that our instruments, now measuring instruments, hear. They may be beatified by their miracles—who would deny it to St. Penicillin or St. Morphine? Or, more lowly, they may be as beautiful as the ten billion pounds of phosphoric acid, H_3PO_4, manufactured every year. You're more likely to have heard of the rougher guys, the spectacular hydrochloric, nitric, and sulfuric siblings. But this quiet one is responsible for a good part of the essential phosphorus in your DNA.

Perhaps it's time to stop here and take another tack. Let's posit that we've discovered in this anthropological study of chemistry a reliable sampling of the qualities the experts/natives use as attributes of beauty. Chemists have an aesthetic. Maybe we don't call any molecule ugly, but some molecules are more beautiful than others. Does 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?

A fundamental problem underlying this question, 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 doesn't fit into the existing (fashionable?) aesthetic frameworks erected by philosophers.

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 on the part of the viewer (listener, etc.) a degree of detachment from his surroundings, and the elements of intensity, unity, and complexity in the object viewed *(6)*. His argument deserves deeper exposition than these fuzzy 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've

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seen more detached than chemists looking at molecules are computer hackers or Pachinko players. Intensity has been discussed above in the context of structure 1. That molecule 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 are 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 hemoglobin 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 running through the tokens of chemical beauty that inclines me to another aesthetic philosophy, that of Nelson Goodman *(7)*. 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 $NaNb_3O_6$ 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 hemoglobin does, therefore I care about it. And the molecules in this Marginalium 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 *(8)*, saying that X is beautiful is almost the dullest thing one can say about X. One needs to describe the object's attractiveness.

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—hemoglobin like a fern unfurling, 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.

References

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