densities with increasing time as the Universe evolved. He relates this curve to the creation of complex structures through the bifurcations characteristic of systems far from equilibrium, together with a generalized principle of natural selection.

Grand schemes stand or fall by their ability to deal with the details of the broad themes they are supposed to synthesize. Although the book covers much material in an enlightening way, I sometimes found it disappointing in this respect. The discussion of the anthropic principle tilts at a straw man that I do not think anyone would seriously espouse. This nice discussion of the important theme of entropy does not explicitly recognize the major unsolved problem of gravitational entropy, although he lays the groundwork to do so. His definition of life is inadequate in that it simply fails to comprehend the full complexity of biochemical systems, and his principle of natural selection is vague and verging on the tautologous.

Finally, how successful is Chaisson in producing the overall integration he intends? The energy-flow issue he focuses on is an important adjunct to the growth of complexity but is not, in my view, the central feature that makes it all possible. High energy-flow density is a requirement, but so are the accumulation of information, for example, and the growth of the ordered structures that make this possible. Indeed, his approach has no real capacity to characterize truly complex systems possessing massive hierarchical ordering, as opposed to less complex but very energetic systems such as the flame of an acetylene torch. The approach might perhaps have been given more substance by relating it to network thermodynamics in complex, hierarchically structured systems, but that has not been attempted here.

Finally, 'grand syntheses' also vary in their degree of ambition, and here Chaisson verges on dangerous territory. His professed aim is to include "all known manifestations of order and complexity in the universe". He wishes, for example, to include cultural evolution in his grand synthesis and to espouse "a new philosophy — a scientific philosophy". But his new philosophy does not touch truly human concerns such as aesthetics, ethics and human culture in a serious way. Nor does it even begin to probe how human cultures deal with the grand themes of life — fear and hope, war and peace, love and death. The grand claims to deal with cultural evolution and to provide a new philosophy are, in the end, not fulfilled — but the journey is interesting and thought-provoking, and the book will serve a useful purpose if it encourages others to think in a synthetic way. ■

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## Science in culture

### Volumetric valencies

**The molecular visualization tool devised by Preston MacDougall and Christopher Henze.**

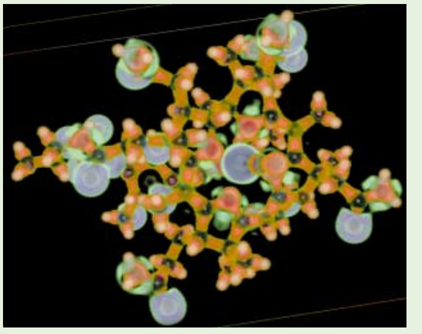
*Martin Kemp*

Our desire to see what the building-blocks of nature look like seems to be irresistible, even when it is meaningless to talk of their visual appearance in any normal sense. Of all the modern genres of representing the unseeable, none has offered a more beguiling parade of visual delights than the modelling of big molecules. From the polished glyptic formula kits of the nineteenth century to today's proliferating programs of computer modelling, the images have not only satisfied our cognitive urges but have also played key roles in understanding and predicting the properties of molecules that are operating at the very heart of life, disease and death.

As the now quaint-looking ball-and-stick constructions have been superseded by a range of computer programs, such as Per Kraulis's widely used MolScript, so it has become apparent that different modes of representation may highlight quite different kinds of structural information. Accordingly, each system of modelling can handle potentially different aspects of the properties of the molecule. The as-yet-unwritten history of the iconography of molecules would tell of complex symbioses between new kinds of information, new and old representational means, and the research questions that shape the visual grammar of the imagery.

One of the most beguiling of the new systems is that recently devised by the chemist Preston MacDougall, of Middle Tennessee State University, and Christopher Henze, a visualization specialist at the NASA Ames Research Center in California. Their images are based on the topological analysis of the distribution of electron probability density, the cornerstone of Richard Bader's quantum theory of atoms in molecules. Using the laplacian of the probability distribution, their models effectively plot the lumps and hollows, the extrusions and holes in the electron cloud around each nucleus. The resulting sculptures could be described as the joint handiwork of classical and quantum agents.

A fourth dimension is provided by the colour coding, in which a rainbow colour scale is taken as corresponding to a range of charge concentration, from 'cool' blue depletions to 'hot' red concentrations. The transition from green to yellow corresponds to the inflection between depletion and concentration, and white denotes the very highest concentrations. Even with this amount of modelled and coloured information, the static image of an elaborate molecule remains frustratingly complex to unravel. The process of visualization is completed by an animated fly-around facility and by an opacity-function editor that allows



**MacDougall and Henze's image of the vitamin $B_{12}$ complex (cyanocobalamin form) is the joint handiwork of classical and quantum agents.**

us to focus and re-focus interactively on features of special concern (see *Theor. Chem. Acc.* **105,** 345; 2001).

The tangibly seductive nature of the tool is not in doubt. But is all the ingenuity worth the effort in scientific terms? The answer is a definite yes, in that it represents an extension of the power of three-dimensional models to predict chemical bonding. Not only do the lumpy configurations reveal very clearly the strong covalent bonding that provides the structural integrity of a molecule, but they are also very effective in denoting sites of noncovalent interactions, the weaker links that typically involve hydrogen atoms at the extremities of large molecules. The plastic modelling tool discloses topologies that permit the identification of reactive sites, including novel ones that are outside the purview of rule-based algorithms. The identification of such sites promises rich potential, most notably in drug design.

As MacDougall himself recognizes, the historical antecedents of such techniques of sculptural 'fitting' go back at least to the 'lock-and-key' model of substrate binding advocated by Emil Fischer at the end of the nineteenth century. There is even an echo of the ideas of Nicholas Lemery, author of *Cours de chymie* in 1675, who was once derided for his conjecture that "chemical combination between two substances, such as an acid and a base, might be accounted for by supposing that the particles of one were sharp,and those of the other porous, and that chemical combination was effected by the fitting of the points into the holes".

There is a nice sense that with the new tool, as is so often the case in scientific visualization, fundamental kinds of visual satisfaction and scientific functionality nourish each other in equal measure. For the animated fly-around, see www.nas.nasa.gov/~chenze/Preston/b12.mpg ■

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