Mackay, Alan L. (1997) Lucretius or the philosophy of chemistry. *Colloids and Surfaces A: Physicochemical and Engineering Aspects* 129-30, 305-310.

# Lucretius or the Philosophy of Chemistry

Alan L. Mackay

Dept. of Crystallography, Birkbeck College, (University of London),
Malet Street, London WC1E 7HX., U.K.

**Abstract**

A world view deriving from the objective knowledge acquired by the physical sciences is contrasted with the fashionable subjective philosophical view that all systems of thought are equally valid ways of structuring the universe. As Lucretius guessed, atoms are real and are not simply arbitrary constructs to explain the observations. Mathematics and computing have an important role in permitting long and sophisticated arguments to be carried through.

Reinhard Nesper (of ETH, Zürich) has remarked[1] that there is no philosophy of chemistry, although there is a philosophy of physics[2]. This observation merits expansion[3]. A philosophy of chemistry[4] (as that of physics) must be a sub-set of a general philosophy or *Weltanschauung.* A philosophy of chemistry looks predominantly at a particular hierarchic level of the world, that concerning atoms, and it looks with the tools of chemistry, which nowadays include the electron microscope, X-ray diffraction and NMR, which enable us to see individual atoms directly for the real objects they are[5], rather than as the concepts or constructions of a particular society, as the views of certain present-day observers of the activities of scientists would have it[6]. 'Atom' is not a philosophical term like 'justice'.

The first philosopher of chemistry, the inheritor of the outlook of Democritos, inventor of the concept of atoms[7], whose works were suppressed by Plato and have not come down to us directly, was perhaps

---

[1] Personal communication.

[2] German culture seems to require a 'philosophy' although people in England can do without one.

[3] The title is modelled after the remarkable series of short essays, "Today and Tomorrow", produced by Kegan Paul, Trench, Trubner and Co. in the 1920s with titles such as "Daedalus or Science and the Future" (by J. B. S. Haldane).

[4] An example of a philosophy of chemistry, or at least of the philosophy of a chemist, is furnished by P. W. Atkins' book, "The Creation", (1981).

[5] W. H. Bragg, with his 'picture' of the arrangement of atoms in diopside (Z. f. Krist., **70,** 488, 1929), might be said to have been the first to 'see' atoms (with a synthesised picture), but the definition is somewhat arbitrary and atoms had been 'seen' less directly much earlier.

[6] History of the Human Sciences, **8,** (2), 91-129, (May 1995).

[7] The Vatican Council ruled (in 1870) that "If anyone shall not be ashamed to assert that, excepts for matter, nothing exists; let him be anathema". Similarly, in India, Sarmad Shahid (Sarmad the Martyr, whose tomb is at the gate of the Jama Masjid in Delhi) said of the standard declaration which all Muslims make ("There is no god but Allah"), that he could subscribe only to the first part, and was immediately executed by Jehangir.

Lucretius (first century BC) who set a goal, at which we should all aim, of producing a world view which would include everything, from primeval atoms to the cosmos, in a consistent whole. A philosophy is rather like a coherent edifice of bricks and mortar. The bricks represent the stubborn facts of observational and experimental science embedded and held in the correct relative positions by the adjustable mortar of society, culture and language. Philosophy concerns itself with fundamental questions (or pseudo-questions) about meaning, language, logic, perception, consciousness, properties, space and time, as well as more nebulous issues of God, the soul, freedom, morality, aesthetics, etc.

There is a philosophy of physics because, at the levels of quantum mechanics, relativity, and cosmology, physics *is* actual philosophy and traditional discursive philosophy has nothing to add, because introspection[8] and looking at the chairs and tables which are the familiar equipment of philosophers, tells us nothing about the microworld nor the macrocosmos, which are on scales (in space and time) beyond those of our everyday experience. In Scotland, physics is (or at least was) called 'natural philosophy' and indeed physics *is* natural philosophy, the word *philosophy* having been usurped by modern sophists such as Roger Scruton who, for example, admits that "The study of space and time is complicated by the intrusion of physics"[9]. Alain Aspect's experimental demonstration of non-locality - that every part of the world is connected to every other - has superseded the paradoxes of Zeno on which philosophers have spent too much time. Even the apparently simple concept of the vacuum of space is much more complicated than it might appear and vacuum fluctuations can be physically important being, for example, involved in the production of light by collapsing bubbles, an effect visible to the naked eye and, less apparently, in the mutual attraction of two plates in the Casimir effect[10].

At the greatest distance from fundamental physics we observe the distinctively human structures of languages, religion, money, art, morals, law which had no existence before the advent of human beings. These are structures in the *noösphere*[11], created by human beings to assist in the operation of societies although, of course, they have material consequences and reside in and are transmitted as artifacts.

Mathematics is an intellectual structure of a different type. It appears to be a logical system existing in the noösphere independently of human beings, but discovered by them, spun out of a few premises. Starting with

---

8 Every week, PET (positron emission tomography) of the human brain is telling us more and more about how we think and how different intellectual tasks are disposed in the brain.

9 R. Scruton, "Modern Philosophy", Sinclair-Stevenson, London, (1994). p. 571.

10 See, for example: "Twentieth Century Physics", ed. L. M. Brown, A. Pais and A. B. Pippard, Inst. of Physics Publishing , Bristol and American Institute of Physics Press, New York, (3 vols. 1995).

11 We find that the concepts, introduced by Teilhard de Chardin and V. I. Vernadskii, of *geosphere, biosphere, noösphere* to be most useful. To these should now be added *genosphere,* the world of genetic sequences.

certain postulates many consequences of these postulates can be generated. The simplest are the relationships between the integers - *"Die ganze Zahl schuf der liebe Gott; alles Übrige ist Menschenwerk" (Kronecker).* Relationships between the integers can be brought into correspondence with relationships between objects and quantities in the real world and accountancy began very early. However, the integers do not explain everything and the discovery in Greek times that the diagonal of a unit square was irrational came as a shock. It was surprising that asking for the square root of two could generate an infinite, non-repeating sequence of numbers[12]. This shock has been paralleled in our own times by the discovery[13] of the Mandelbrot set, where the recurrence z := z^2 + c gives patterns of infinite complexity. There is a close, but perhaps not exact, correspondence between mathematical relationships and physical measurements, which is extremely useful in following through the consequences of hypotheses. Mathematics enables us to carry through extremely elaborate arguments in spite of the inadequate capacities of our brains[14] and computers have greatly augmented this ability[15]. Mathematics gives results of apparently infinite accuracy. For example Pi can be calculated to a million digits, although the ratio of circumference to radius of any physical circle would be affected by the curvature of the space in which it is embedded due to gravitating objects in the universe. The distinction made in computers between integers and real numbers reflects the cleavage between mathematics and physics. The nature of mathematics is indeed a matter for philosophy, but is not our main concern here, although the relationship of mathematics to the physical world is most important. Paradoxes of mathematics, such as those associated with Gödel's Theorem, occupy philosophers, but chemists and physical scientists who use mathematics as a tool, are well aware that, as for other tools, it can be wrongly used and bring injury to the user. We must return (below) to the relationship of mathematics with chemistry but, just as it is useful for the chemist to ask the mathematician for help, so it is legitimate for the mathematician to ask the chemist whether the various structures he may conjure up from his symbols may have any physical significance. Has Riemann's zeta function any connection with chemistry[16]? Mathematics is simply the investigation of structures in the noösphere but with applied mathematics one returns to the real world with suggestions as to how real matter may behave. At the earliest stage Euclid's "Elements" (including the

---

[12] The Babylonians could calculate the square root of two to an indefinitely great accuracy. Ed Fredkin has discussed the possibility that space may be granular and that, like a computer, only a limited number of digits of information can be stored in a given volume (see: R. Wright, "Three scientists and their gods", Times Books, New York, (1988)). The concept of the Planck Length points in this direction.

[13] The Mandelbrot set was a discovery, not an invention.

[14] 'Can you do addition?' the White Queen asked. 'What's one and one and one and one and one and one and one and one and one and one?' 'I don't know', said Alice, 'I lost count'. (Lewis Carroll).

[15] The computer programme *Mathematica* (S. Wolfram) should be particularly mentioned as augmenting human abilities.

[16] It involves summing series such as those involved in calculating the potential in a lattice. See, for example: B. W. Ninham and S. Lidin, Acta Cryst., **A48,** 640-649, (1992).

books 14-15 added later) was a guide to the geometry of space and in particular it provided the five regular Platonic Solids as ideal objects which might be seen in imperfect form in the real world. Today there is an infinitely greater range of possible abstract forms some of which may be realised in practice. Einstein wrote: "The human mind has first to construct forms, independently, before we can find them in things." This is part of the role of mathematics.

Chemistry we may take to be the level of organisation of matter between that of fundamental physics and that of biology, where the language of DNA begins, although increasingly chemistry shades into biochemistry. Chemistry is concerned with the organisation of atoms into larger units. Before the discovery of atoms chemistry could have no adequate predictive theory and thus it is not necessary here to consider the history of alchemy and chemistry, significant and interesting though this may be. Mendeleev, with his organisation of the elements into the Periodic Table, was one of the first to make important predictions. There were many insights like that of Democritos. For example, chemistry is characterised by structure and by change. Heraclitus' (ca 550 - ca 475 BC) aphorism "everything flows", was superseded by the Principle of Le Chatelier (1888) "everything flows downhill". Before van't Hoff, who postulated (1874) the tetrahedral carbon atom and that chemical compounds had actual structures in three-dimensional space, there was only a steady accumulation of facts which formed a random heap with some fragments of regularity rather than an organised edifice. The philosophy of chemistry began when Lucretius began to organise what facts he had into a coherent recognisable building. Alchemy was a fanciful baroque structure which collapsed under its own weight. However, Lucretius' view of the world conflicted with that promulgated by dogmatic religion and was largely suppressed[17].

Chemistry is concerned with the combinations of atoms. With about 100 different kinds of atoms the number of compounds is very large and chemistry deals primarily with the topology of the corresponding configuration space and how to move about in it. The philosophy of chemistry then involves N-dimensional geometry. Each compound is metastable and resides in a local minimum in this configuration space. The topology has been approached, for example by René Thom's *catastrophe theory*, with the classification of singularities. C. H. Waddington too, in developing theoretical biology, has made familiar the concept of an

[17] Quite recently the Vatican has again raised the question of trans-substantiation (the transformation of wine into blood and bread into flesh in the Mass - *hoc est corpus* - which gave rise to the vulgar expression *hocus-pocus*) by ruling that wheat gluten is the active principle in the ceremony and that priests who are allergic to gluten cannot properly participate. Rice gluten is deemed to be an invalid substitute. (see: The Guardian, 10/10/95 and Nature, **381,** (27 June 1996)). Curiously, the latter reference comments on "the unlikely similarity between titin (from muscle) and glutenin (from wheat flour)".

It has been suggested by P. Redondi in his book "Galileo - heretic" (English edn. 1988), that the real crime of Galileo was that of atomism and that, since this issue was dangerous to the doctrine of trans-substantiation, it was dropped in exchange for a plea of guilty on the issue of heliocentrism.

*epigenetic landscape* which is something like the table of a pin-ball machine. The signal discovery of our generation has been that of the genetic code. This has revealed that there is a natural language and that one structure made of atoms may bear a relationship to another structure made of atoms that a description in a natural language may bear to an object. The DNA corresponding to a protein sequence is a label describing the position of the protein molecule in configuration space - the address of the local minimum - and enables us to reach this minimum directly, without having to tilt the configuration space, as a skilled operator might tilt the pin-ball table (for example by changing the temperature) to get the ball into a winning hole.

Chemical structures are hierarchic, that is, levels of organisation can be distinguished which are partially separable. Chemistry today is pressing on to higher levels and is becoming a science of growth and form at the molecular and macromolecular levels. In considering levels of organisation the largest jumps occur in going from atom to molecule and from molecules to cell. Hierarchic levels are only approximately separable and, as Aspect's experiment shows, everything in the Universe is coupled to everything else. If you torture Nature (as the philosopher Francis Bacon tortured human prisoners) and force answers to cunningly posed questions, it can be shown that the quantum picture of the world obtains at all levels and fits observations better than the Newtonian picture and often to an astonishing accuracy. Sometimes questions demanding the answer yes or no can be formulated to which Nature clearly replies that the quantum picture is the better one. The world of quantum mechanics is quite unfamiliar to people who live on the scale of human beings and could not be deduced by reflection, but only by extremely subtle experiment. Even in the simplest case, since the wave function of two electrons is not just the linear sum of that of each electron separately but contains a cross term, quantum mechanics shows how a system is not just the linear sum of its separate parts. Questions such as this, and the consequences of the exact identity and thus indistinguishablity of two electrons are basic to actual philosophy.

Chemistry is characteristically concerned with the collective behaviour of atoms, each of which has its own properties but which interacts with others. Quantum mechanics governs this individual and collective behaviour. Measures which are statistical in nature, such as temperature, volume and density, emerge. In many places there is still a duality between wave and particle, between discrete and continuous descriptions. Thermodynamics is entirely concerned with statistics. Questions of *qualia* (is an atom green; is a chlorophyll molecule green; if we were all blind would a leaf be green?) which pre-occupy philosophers are largely illusory and are steadily becoming clearer with the application of more subtle methods to the examination of the operation of human sense organs and the brain. The paradigm of the deterministic machine, based on the clockwork of the period, started by La Mettrie with "L'Homme Machine" has now been replaced by far more sophisticated understanding.

The three areas - nanotechnology, (the physical fabrication of very small structures), macromolecular chemistry, and the generation of various ordered structures by living organisms[18], are rapidly approaching each other as science advances. "Growth and Form", (the title of D'Arcy W. Thompson's influential book of 1916), is becoming more topical.

There has been a corresponding rise in activity to provide mathematical, primarily geometrical, tools and models for the understanding of structures which are more general than those of crystals. The formalism of crystallography is essentially complete and the 230 crystallographic space-groups of symmetry furnish a complete description of the ways in which identical (asymmetric) units can be arranged in space so that each has identical surroundings. However, particularly after the surprise appearance of quasi-crystals, it has been realised that there are more general structures, composed of units of a few types, which are outside the framework of orthodox crystallographic theory. In these the units may be in only approximately identical (quasi-equivalent) positions. Crystallography still does not have a very satisfactory mathematical formalism for the treatment of change. The objectives and outlook of Joseph Needham[19], J. D. Bernal, C. H. Waddington and the other members of the Club for Theoretical Biology in Cambridge in the 1930s, which included the establishment of an institute for physico-chemical morphology[20], have become very timely. General questions of complexity and the emergence of properties are matters of philosophy which mathematics can illuminate.

The key question of the relationship of mathematics to physical structure is best understood through the concept of projection, taken in its most general meaning.

'Reductionism' is now used chiefly as a fashionable depreciatory label[21], being contrasted with 'holism'. It is supposed to regard human beings as 'just atoms'. However, the world is simply too complicated for everything to be taken into account at once. It is possible only to select some problem, to decide what factors are the most important and to neglect the rest. Possible factors must include ourselves and our interactions with the world. In mathematical terms we set up the whole matrix of the interactions and take the space of the eigenvectors

[18] See particularly: S. Mann, "Biomimetic Materials Chemistry", VCH, (1996).
[19] Joseph Needham's essays of 1936 "Order and Life" (MIT Press, 1967) are still important and stimulating.
[20] An unsuccessful application was made to Warren Weaver and W. E. Tisdale of the Rockefeller Foundation.
[21] The Ham and High (a London newspaper) recently carried a photograph of Lewis Wolpert labelled 'the well-known reductionist'.

corresponding to the first few largest eigenvalues. This is impossible, because we would have to know everything about the system first. We can only select what seems important and then, if the model does not represent reality sufficiently closely, try again with a different selection. Every organism has inside itself a model of the external world and of itself with which it operates.

The process of reducing the number of the dimensions of the space with which we have to operate is 'projection'. The clearest mathematical description of projection is that involving the generalised inverse of a matrix or singular value decomposition[22] which describes explicitly what information is retained and what is lost. Restoring ('resurrecting') an object from its projection is impossible, since information has been lost and it is necessary to restore this information from our external experience and knowledge. The description of something in a natural language is a projection and to restore the scene requires that that we supplement the language with what we already know.

In order to present a situation in mathematical form many features must be neglected and we can only choose a few factors which we consider to be important. We can then manipulate the mathematical description to reveal hidden relationships and finally restore the result to the real world for comparison with the complete situation. If we have chosen our direction of projection correctly then the results may be significant for the real world and may be used to assist our choice of actions in the real world.

Chemistry shades into biology and into general systems theory[23]. In the genetic code we see, for the first time, the existence of a natural language, like the natural languages of speech, where symbols "stand for" other objects. In the case of the genetic code, there is the very severe restriction that both object and symbol are made of atoms and must follow the laws of atoms. With the development of the conscious design of guest molecules and templates for building inorganic cage structures, chemistry moves in the direction of a 'genetic code' for the synthesis of inorganic materials. One molecule may 'describe' another and a template for a molecule is effectively its address in configuration space[24]. We see a convergence between the storage of arbitrary information by 'writing in' to microstructures and the specialised roles which different templates may

---

[22] See: W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, "Numerical Recipes", (2nd. edn.), Cambridge University Press, (1992) for an excellent description and for actual programmes.

[23] For example: L. von Bertalanffy, "Problems of Life", (1924) and "General System Theory" (1968), A. J. Lotka, "Elements of Mathematical Biology" (1924), (Dover, NY, 1956), C. H. Waddington (ed.), "Towards a Theoretical Biology", L. L. Whyte, A. G. Wilson and D. Wilson (eds.), "Hierarchical structures", American Elsevier, New York, (1969), etc.

[24] One might well ask: "Where are the genes for Paulingite?" (title of a lecture by A. L. Mackay, Lund, 20 March 1984).

have in the synthesis of complex compounds. The recognition of hierarchic structures in quasi-crystals has broadened the horizons of what is possible. Many questions arise about the origin of life and the evolution of the genetic code, the operation of the brain, etc. but all these are to be answered by the methods of science rather than from the ruminations of academic philosophy. Serious philosophical questions arise at the level of chemistry.

Thus, we conclude that there is a philosophy of chemistry[25], the *Weltanschauung* of people who deal with atoms, individually and collectively[26], and that if philosophy is indeed the examination of the roots of our intellectual system, it should begin with the physics, chemistry and biology which are the basis of our physical existence. A general philosophy, which is not founded on science and neglects chemistry, cannot be a philosophy at all, but only a castle in the air, like the various *revealed* religious systems, the designed legal systems, the evolved social systems, and such like. As E. O. Wilson put it: "The history of philosophy consists largely of failed models of the brain".[27]

---

[25] Friedrich Engels (1820-1895), especially in his "Dialectics of Nature", attempted to absorb chemistry into his general philosophy. He was much influenced in this by his friend Carl Schorlemmer, the first professor of organic chemistry in Britain, who studied how the properties of analogous hydrocarbons change with increasing numbers of carbon atoms. This led directly to Engels' phrases about the 'transformation of quantity into quality' which became a mantra of dialectical materialism.

[26] The adverbs apply both to 'people' and to 'atoms'.

[27] "Naturalist", (1994).