



Dædalus

Journal of the American Academy of Arts & Sciences

Fall 2014

From Atoms to the Stars

Jerrold Meinwald	Introduction 5
Christopher C. Cummins	Phosphorus: From the Stars to Land & Sea 9
John Meurig Thomas	Foresight, Unpredictability & Chance in Chemistry & Cognate Subjects 21
Fred Wudl	The Bright Future of Fabulous Materials Based on Carbon 31
Chaitan Khosla	The Convergence of Chemistry & Human Biology 43
K. N. Houk & Peng Liu	Using Computational Chemistry to Understand & Discover Chemical Reactions 49
Jeremiah P. Ostriker	From the Atom to the Universe: Recent Astronomical Discoveries 67
Anna Frebel	Reconstructing the Cosmic Evolution of the Chemical Elements 71
Gáspár Áron Bakos	Exoplanets, 2003 – 2013 81
Michael A. Strauss	Mapping the Universe: Surveys of the Sky as Discovery Engines in Astronomy 93
Scott Tremaine	The Odd Couple: Quasars & Black Holes 103
Pieter van Dokkum	The Formation & Evolution of Galaxies 114
David N. Spergel	Cosmology Today 125

Introduction

Jerrold Meinwald

JERROLD MEINWALD, a Fellow of the American Academy since 1970, is the Goldwin Smith Professor of Chemistry Emeritus at Cornell University. His research has contributed to a wide range of chemical and chemical biological subjects, including organic photochemistry, reaction mechanisms, the synthesis of chiral inhalation anesthetics, natural product chemistry, and chemical ecology. His publications include the edited volumes *Chemical Ecology: The Chemistry of Biotic Interaction* (with Thomas Eisner, 1995) and *Science and the Educated American: A Core Component of Liberal Education* (with John G. Hildebrand, 2010). He is Secretary of the American Academy and Cochair of the Academy's Committee on Studies and Publications.

Why “From Atoms to the Stars”? In the Summer 2012 issue of *Dædalus*, entitled “Science in the 21st Century,” May Berenbaum and I sought to provide representative accounts of recent progress in the natural sciences. But it turned out that two areas of the physical sciences – astronomy and chemistry – cried out for more extensive attention than we were then able to provide. Consequently, Jeremiah Ostriker and I recruited a group of outstanding astronomers and chemists to write a set of essays to complement this earlier issue. Each of the new essays in this volume discusses important scientific developments in astronomy and chemistry in specific areas of study to which the authors themselves have made major contributions.

Philosophers, alchemists, and subsequently chemists have examined the properties and transformations of matter in all its diversity for over two millennia. The pace of progress of these studies (and, in fact, in all areas of science) picked up markedly toward the end of the eighteenth century, and has been increasing rapidly ever since. It was not until twenty years after the first performance of Stravinsky's *The Rite of Spring* (and, I was shocked to realize, during my own lifetime!) that it became clear, with James Chadwick's discovery of the neutron in 1932, that all ordinary matter is made up simply of protons, neutrons, and electrons. While protons and neutrons were at first believed to be the fundamental particles making up atomic nuclei, they have since the 1960s been best understood as *composite subatomic*

Introduction particles, each made up of three inseparable quarks. Protons (which carry a single positive charge) consist of two *up quarks* and one *down quark*. Neutrons (electrically neutral) comprise one up quark and two down quarks. Interestingly, this revolutionary structural insight into the nature of matter has had no impact at all on our understanding of chemistry.

The simplest atom, hydrogen (H), which is not only the most abundant form of ordinary matter in the observable universe but also the most abundant atom in our own bodies, consists of a single nuclear proton and a single planetary electron. The addition of one or two neutrons to the proton yields the hydrogen isotopes deuterium and tritium, respectively. The combination of two nuclear protons and two neutrons, along with two planetary electrons, produces an atom of helium (He). With the exception of tiny amounts of lithium (Li), whose nucleus contains three protons, these are the sole types of atom produced as a consequence of the Big Bang some 13.8 billion years ago. From a chemist's viewpoint, there are some extremely important differences between hydrogen and helium atoms. Hydrogen atoms are able to bond to many other types of atoms to form stable molecules such as elemental hydrogen (H₂), water (H₂O), ammonia (NH₃), methane (CH₄), and literally millions of other "organic" compounds (all of which also contain carbon). Helium atoms, in contrast, prefer to remain alone.

It was not until the mid-nineteenth century (1869) that Dmitri Mendeleev taught us that all the known elements, when listed according to increasing atomic number (the number of protons in the nucleus), could be arranged into a "periodic table." His table revealed that the fewer than one hundred naturally occurring elements fall into periodically recurring groups (such as noble gases and halogens), a finding that enabled him to predict (correctly) the ex-

istence of unknown "missing" elements that remained for future research to discover. Our understanding of how, where, and when all the elements with an atomic number greater than two (quaintly referred to as "metals" within the astronomical community) were produced is much more recent and still somewhat incomplete. Anna Frebel's account in this volume of the origin of these elements following the Big Bang is a fascinating story that is much less well known (even among chemists) than it deserves to be. Her essay (among the astronomy contributions) provides an ideal introduction to the very existence of chemistry and of life itself.

Christopher Cummins responded to our invitation to write an essay on inorganic chemistry by examining the chemistry of a single element: phosphorus (P). In his exploration of phosphorous, we learn that pyrophoric (spontaneously combustible) elemental white phosphorus consists of discrete P₄ molecules in which each phosphorus atom occupies the vertex of a tetrahedron, the simplest of the five Platonic solids. (By a striking coincidence, Plato tells us that Timaeus considered the "element" *fire* to be composed of tetrahedral particles!)

Cummins's research on how the synthesis of phosphorus-containing compounds might be greatly simplified exemplifies theoretical and experimental chemical thinking at its best. From a consideration of the complex genesis and low abundance of phosphorus in the universe (where it is relatively rare) and in living organisms (where it occurs in concentrations much higher than it does in our solar system), we move on to accounts of its vital importance in agriculture and industry.

Tracing the passage of phosphorus from the soil into plants, then into animals, and finally into the sea illuminates some seriously underappreciated ecological con-

cerns. The sad tale of the rise and fall of the chemically innovative Canadian research project that aimed at improving agricultural phosphorus use by creating a breed of pig, the *Enviro-pig*, able to digest plant-derived phosphorus compounds in its diet better than any previously existing breed of pig, brings this essay to a close. It may come as a surprise that the study of a single element reaches into such a wide range of human concerns, spanning agriculture, industry, the health sciences, ecology, and even the social sciences. Readers of Cummins's essay will be rewarded not only with insights into some beautiful science, but also with extensive material for chemistry-based cocktail party conversation.

The borders between the classical scientific disciplines are rapidly disappearing, but continuing in the more or less traditional fields of *inorganic* and *physical chemistry*, John Meurig Thomas has given us an intriguing essay on chemical catalysis, embedded in a wide-ranging examination of the importance of unpredictability and chance within and beyond chemistry. His vision of the "chemist" leans in the direction of what used to be termed "natural philosopher." He provides a refreshing view of the world of chemical research, with an emphasis on the importance of entirely unanticipated discoveries and unforeseen practical applications. His case studies serve to remind us of the remarkable value of curiosity-driven research. There is an important message here for society at large with respect to shaping the most productive science policy.

The discipline of chemistry has quietly undergone an absolutely remarkable transformation (or perhaps expansion would be a better term) over the last half-century. This development has manifested itself in part through the examination of biology as a molecular science. With our increasing understanding of the chemistry of proteins,

nucleic acids, and the myriad "small molecules" that serve as molecular messengers throughout nature, dramatic and even unimaginable improvements in the practices of medicine (including psychiatry) and agriculture are certain to play a prominent role in the twenty-first century. In another direction, with the successful synthesis first of the simplest organic molecules (urea, ethyl alcohol, vanillin) and then of many of the much more complex structures (cholesterol, vitamin B-12, insulin) far behind us, can the construction of synthetic viruses and even living cells be far off?

Another major opportunity for research that is occupying the attention of many contemporary chemists is the development of *materials science*, an area discussed in Fred Wudl's essay. As a result of many advances in physics, we know vastly more than we did only a few decades ago about the way atomic and molecular interactions influence the macroscopic properties of all sorts of materials. We know why some materials are brittle, flexible, good electrical conductors, good electrical insulators, magnets, or light emitters or absorbers. As the physics of all these phenomena is better understood, it becomes possible for chemists to design and produce new materials from which everything from "improved" fabrics to computers, airplanes, and televisions can be made. Quite remarkably, the element carbon plays a central role in the design of many of the novel materials with desirable properties, such as "self-healing" plastic (vitrimers) or solar photovoltaic cells. Wudl's essay outlines how this area of chemistry evolved and what we may expect from it in the decades to come.

Chaitan Khosla has focused his essay on the field that has become known as *chemical biology*. Perhaps influenced by the ancient Greek aphorism "know thyself," he places particular emphasis on the roles that chemistry plays in understanding (as

well as improving) the lives of *Homo sapiens*. Chemistry lies at the heart of much medical research, from the development of noninvasive imaging techniques such as MRI and PET scans to the discovery of new molecular targets that may serve as the basis for the design of much-needed, novel anti-infective agents to help battle malaria, Lyme disease, SARS, and many other threats to human health. In some areas, the chemistry and biology relevant to health is already fairly well understood, and “translation” from theory to application can be expected to proceed smoothly. In others, such as the chemical/biological understanding of brain functioning or the control of development, basic research remains an essential precursor to human applications. Khosla’s essay illuminates a field the chemical basis of which is not yet widely enough appreciated.

Chemistry is an experimental science. Some of its complexity derives from the fact that it deals typically with huge numbers of molecules at a time; after all, an ounce of water contains about 10^{24} H_2O molecules, roughly equal to the estimated number of stars in the observable universe. Nevertheless, the enormous power of contemporary computers, combined with fundamental physical insights provided by the development of quantum mechanics, has resulted in the birth of computational chemistry, which provides both explanations and predictions of chemical properties and behavior. K. N. Houk and Peng Liu describe examples of the power of computational chemistry in predicting the products of chemical reactions, in understanding the course of newly discovered catalytic reactions, and even in designing synthetic enzymes capable of catalyzing reactions for which no natural enzymes exist. Although the power of computational chemistry is now apparent, the science is still in its infancy.

The world of computational chemistry is a far cry from the chemistry labs of our youth, with their litmus paper, Bunsen burners, and distilling flasks. The pungent odors of bromine or nitrobenzene, the beauty of deep-purple potassium permanganate crystals, the brilliance of burning magnesium, the eerie blue glow of luminol treated with hydrogen peroxide (experiences that have attracted generations of young students to chemistry in the past) are absent from this new world. They are replaced by the less sensual but nevertheless deeply satisfying insights that only the computer can give! There can be no doubt that much of the sort of chemical research that is now being carried out in the conventional laboratory with actual chemicals will be done within the next few decades faster, cheaper, and more safely by computational chemists sitting in their offices.

In summation, what we have here is a five-course chemical tasting menu. It would have been possible to choose five entirely different aspects of chemistry that would have given an equally appropriate account of the rapid advance of this lively discipline. In many menus, some of the courses or wine-pairing descriptions use unfamiliar terminology. Understandably, we are inclined to avoid incomprehensible or unpronounceable items. Describing chemistry presents an analogous challenge; one of the great problems in writing about science is how to eliminate jargon. But this difficulty can be readily taken care of these days simply by googling the obscure terms (Wikipedia also offers highly informative accounts of everything from the Platonic solids, neutrons, the periodic table, and phosphogypsum to the Enviropig and PET scans). Whether chemistry always intrigued you, or whether it was your worst subject in high school, I hope you will find yourself enjoying what our dedicated authors have to say. *Bon appétit!*