The future of chemistry

Chemistry is a very old discipline, with references to chemical transformations and debate about the nature of matter dating back to the times of the ancient Egyptians and Greeks. Modern chemistry began to emerge from alchemy in the seventeenth and eighteenth centuries, thanks to scholars such as Boyle and Lavoisier, leading to rapid advances in the following two centuries. In this feature, eight leading chemists with a broad spectrum of interests look to the future and share their vision for how their own fields may develop in the coming years. Even though research is increasingly interdisciplinary, the articles are roughly divided into traditional areas of chemistry. It is interesting to note, however, the key themes that occur in more than one article, including energy and sustainable chemistry. The chemical tools used to investigate biology — and the analytical tools chemists themselves use — are discussed, as well as the synergy between experiment and theory. Structure and bonding are at the core of the discipline, especially inorganic chemistry, whereas using weaker intermolecular forces to assemble supermolecules is a field with much still to explore. To begin, the central place of synthesis in chemistry is emphasized and extended to chemistry's place in science.

Synthesizing our future

Chemistry has a central role in science, and synthesis has a central role in chemistry. **Ryoji Noyori** from Nagoya University considers where synthetic chemists should focus their efforts.

Chemistry attempts both to understand the structures and characteristics of substances in minute details at the atomic and molecular levels, and to create new compounds with desirable properties and functions. One clear direction, both now and in the future, of this core science is to merge with other fields to produce more interdisciplinary science. In view of its significance, chemistry demands the highest level of scientific creativity and insight to explore its limitless possibilities.

With the characteristics described above, chemistry has rapidly expanded into the field of life sciences, as prophesized by James Watson (the 1962 Nobel Laureate for Physiology or Medicine) when he said "Life is simply a matter of chemistry." When DNA was found to have a double-helical structure in 1953, chemistry really began to enter the core region of life sciences. The decoding of the human genome in 2003 led to a new world of chemical science. Thanks to advanced technologies and the diligent work of scientists in many fields, we are now able to elucidate the precise atomic-level structures of large biomolecules such as DNA, RNA, proteins and polysaccharides.

Consequently, the focus of much chemical research has been moving from structure to function. As dynamic interactions between large biopolymers and small organic molecules often control the processes in living organisms, it seems certain that scientists will soon be able to elucidate the chemical mechanisms of cell functions and perhaps even of human thought and memory. We still have few solutions to the problem of creating peaceful human existence, but furthering our understanding of precise biological mechanisms through chemical biology and chemical genomics aided by advanced biomolecular imaging technologies will lead to the discovery of rational and more effective drugs in the post-genome era.

Although the properties of molecules and their assemblies remain unpredictable solely from their constituent elements, the possibilities for atomic and molecular manipulation are unlimited. Chemical synthesis provides a logical basis for the biosciences and materials sciences, and their technological applications. Synthetic chemistry enables the flexible manipulations of elements — we can create value-added substances from abundant natural resources such as oil, coal and biomass. In principle, we can create molecules that have all kinds of properties at will. In view of the very nature of chemistry, its integration with other research fields will have enormous scientific and technological impacts.

> Chemical synthesis has now reached an extraordinary level of sophistication, but there is vast room for improvement.

Looking at the course of human history, we see that man-made substances and materials have played a significant part in determining the quality of life. Although chemical synthesis has now reached an extraordinary level of sophistication, there is still vast room for improvement. Chemical

synthesis must pursue 'practical elegance'[1] — that is, it must be logically elegant but must at the same time lead to practical applications. Many of the stoichiometric reactions used at present, although useful, can and should be replaced by more efficient catalytic processes.

Catalysis has been, and will remain, one of the most important research subjects, because this is the only rational means of producing useful compounds in an economical, energy-saving and environmentally benign way. According to a promotional brochure from the renowned German chemical company BASF, more than 80% of globally produced chemicals are made using catalytic processes. The importance of efficient heterogeneous, homogeneous and biological catalysts[2] is continually increasing. Practical catalysts must enable reactions that are rapid, capable of being scaled up, and selective in the products formed. Molecular catalysts displaying chiral efficiency that rivals or exceeds that of enzymes are highly desirable[3–5].

At the same time, industry demands the development of thermally stable, salt-, poison- and acid/base-resistant synthetic enzymes, because naturally existing enzymes are not robust. Catalysis is thus critical to the production of commodity chemicals and also new substances in research laboratories. In providing a path of lower activation energy, however, it does not improve the ability to conduct endothermic processes, which require the investment of extra energy or the use of special product-separation technology to shift chemical equilibria to favour the formation of a desired product.

There are many reactions that do not work under thermal conditions. To enhance the power of synthetic chemistry, photosynthetic catalysis enabling otherwise energetically forbidden transformations needs to be explored in greater depth. Similarly, current step-by-step organic syntheses must be a combination of all thermodynamically downhill reactions, limiting the overall efficacy. Therefore, cascade syntheses[6], or those that combine multiple components in a single step[7], are particularly appealing. An intricately designed device that can integrate multiple catalysts along with suitable cofactors to achieve this without the necessity of human intervention is a worthy goal.

Ideally, we should aim at synthesizing target compounds with a 100% yield and 100% selectivity and avoid the production of waste. This process must be economical, safe, resource-efficient, energy-efficient and environmentally benign. In this regard, the atom economy[8] and the E-factor[9] should be taken into account. The 3Rs (reduction, recycling and reuse) of resources are particularly important. Such 'green chemistry'[10] is creative and brings about prosperity, and at the same time takes responsibility for society at large. Any efficient chemical processes must also be socially acceptable. Green chemistry is not a mere catchphrase. It is an indispensable principle of chemical research that will sustain our civilized society in the twenty-first century and further into the future. Green chemistry must therefore be promoted and supported by the scientific community as well as by governments, industry, and all other sectors of society.

Science is destined to be more closely involved with society in this century. It should be no surprise that 'Chemistry: the key to our future' is the slogan of the 2010 Chemistry Olympiad, to be held in Tokyo. In contrast, uncontrolled, excessive economic activity based on science and technology has brought with it a range of global issues. Scientists' efforts should be directed towards solving a range of existing or predicted social and global issues associated with energy, materials, the environment, natural disasters, water, food and health. Chemists have an immense responsibility to tackle these problems; however, the prevalent over-specialization in science tends to make it difficult to find solutions because there are usually multiple causes. To remedy this situation, we need a more broadly based science education, which will better equip future chemists to tackle the issues outlined above.

Science is, in principle, objective. But it is human intelligence and endeavour that discover and create scientific knowledge. The scientific world should be borderless; scientists from both advanced and emerging nations — with different backgrounds and values — must cooperate for the survival of our species within the confines of our planet. This is the greatest challenge facing chemists in conducting their research. ❐

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