

## Dimensions of chemical science

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Chemical science is an old subject. Chemistry, in some form or the other, has been practised for several centuries. In countries like India, dyes were used to make clothes attractive at least 5000 years ago. Metallurgical objects such as statues, pillars and weapons were made in many civilizations a few thousand years ago. Although we may consider the practice of chemistry as age-old, modern chemistry itself is not old. It is generally believed that chemistry, as we understand it today, started in the 18th century with Lavoisier when he propounded ideas on chemical combination, stoichiometry and combustion. We, however, knew very few elements in the 18th century. Thus, Lavoisier's periodic table had around 20 elements. It is only in the 20th century that we got to know 114 elements. If the number of elements is taken as a measure, we will have to consider chemistry to be essentially a 20th century subject. If we go to finer details, we come to recognize that new trends in chemistry started after the understanding of the nature of the chemical bond. The first attempt to understand the chemical bond was by G N Lewis in the early 20th century. Lewis wrote the classic paper on the chemical bond in 1916. This was followed by Linus Pauling, who wrote his famous papers and book on the nature of the chemical bond. I would, therefore, surmise that chemistry is a child of the golden age of science which occurred around the 1920s. This is not surprising since X-rays were discovered during this time and quantum mechanics had its birth. The structure of atoms itself was elucidated by Rutherford not long before this period.

One of the main aspects of chemistry that has played a major role in the development of the

subject relates to structure. The faith that structure forms the basis of everything in chemistry developed since the 1930s. Structure includes molecular structure, spectroscopy, chemical bonding, chemical theory and related aspects. The structural basis of chemistry as championed by Linus Pauling became the underlying theme of much of chemical research and chemical education.

I have always been surprised by the fact that it took so long for physical chemistry to be recognized as an integral part of chemistry. Ostwald and Van't Hoff were the early champions of physical chemistry, under whom most American and European physical chemists worked. Pauling was an exception and worked with Sommerfeld who trained all the well-known theoretical physicists including Heisenberg, Bethe and Born. By 1930, the leaders of physical chemistry in the US were Lewis and Pauling. It was in 1934 that the subject had its formal birth. Amazingly, the inorganic chemistry division got formally recognized by the American Chemical Society only in the 1950s.

Coming back to trends and directions, the three main areas of chemistry during the 1960s and the 1970s were structure, synthesis and dynamics. Synthesis of compounds and materials is the main occupation of chemists. The first compound (urea) was made in 1828 by Wohler in Germany. Since then, there have been many advances in the synthesis of molecules and today, chemists can make almost any molecule of any complexity. There have been many great names associated with the advances in organic synthesis, Wilstatter, Robinson and Woodward being the prominent ones. Progress in synthesis owes much

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to the development of physical techniques based on spectroscopy and diffraction. If we compare the number of compounds made before and after 1950, we really see how the number increased by several factors after the 1950s. This is almost entirely due to the availability of methods for quick characterization and structure elucidation.

Dynamics is an important aspect of chemistry, because it tells us how and why reactions occur. Till the middle of the 20th century, one could measure rates of reaction in seconds and in the early 1960s, rates of reaction that occurred in microseconds were determined. Today, we study reactions occurring in femto seconds. The understanding of dynamics of reactions has undergone a big revolution due to better instrumentation and the development of lasers.

Ever since the advent of quantum mechanics, chemists have tried to interpret molecular structure, chemical bonding and other aspects of chemistry on the basis of quantum mechanics. Note that the first book on quantum mechanics was by Pauling and Wilson. Even physicists read this book to learn the subject. Now-a-days, most chemists use the various quantum mechanical methods routinely. Computer simulation has further strengthened the ability of chemists to explain and predict properties and behaviour of chemical systems.

Chemists have always been outgoing in research, although the teaching of chemistry may not have been always progressive. We often have to remind ourselves that molecular biology actually started in 1951 when Pauling discovered the alpha-helical structure of proteins.

To understand the way chemistry has developed, it is useful to recall the report on chemistry produced by the US National Academy of Sciences in 1985. That report mainly emphasized structure, synthesis, dynamics, catalysis and related aspects. There was a mention of materials and a little of biology, but the emphasis was mainly on molecular chemistry. Reaction dynamics got considerable importance in the report and it is not surprising that there was a vast amount of effort in this area in the subsequent period. Even funding of chemistry was influenced by this report. There was a discernible change in the late 1980s when supramolecular chemistry got recognition.

Molecular chemistry was no longer considered sufficient and supramolecular approaches gained increasing importance.

Today, chemists make use of both molecular and supramolecular approaches and work on a number of interdisciplinary areas of chemical sciences. Although chemists have traditionally worked on interdisciplinary areas all through, it has become a way of life in recent years. The most important frontiers of chemistry today are related to biology and advanced materials. It is, therefore, most appropriate that the more recent report of the US National Academy of Sciences on chemistry, entitled *Beyond the Molecular Frontier*, published in 2003, emphasises less on molecular chemistry but more on materials and biology. Contributions of chemists to biology, environment, health and medicine have become so crucial that a majority of the recommendations pertain to these aspects. Similarly, synthesis and development of new materials of desired properties have come to the fore. Every few years, a major discovery of a new molecule or a new material with unusual properties triggers chemical research in a big way. High-temperature cuprate superconductors, mesoporous silica, fullerenes and nanotubes are typical examples. Science and technology of nanomaterials have become an important pursuit of chemists since the last decade.

If I am asked to pick the greatest chemist of the 19th century, I would pick Michael Faraday. Many people consider him to be a physicist, but he was a professor of chemistry. Being a professor of chemistry, he discovered electricity and carried out experiments on electrolysis, magnetism and so on. He was the first one to make nanomaterials and to experiment on the liquifaction of gases, heterogeneous catalysis and superionic conductors. He also discovered benzene.

For the 20th century, there seems little doubt that Linus Pauling is the one. If I am asked whether there will be a person who will change chemistry in a big way in the 21st century, I find it difficult to imagine such a situation. It may be difficult to find one person at the end of the 21st century, because of the way chemistry works today. Whatever it may be, chemistry will continue to be dynamic in scope with many new frontiers to conquer in the years to come.