Public Lecture Series

CHEMISTRY: BETWEEN THEORY AND APPLICATION

Kehinde Onwochei Okonjo

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Corporate & Public Affairs Department
Covenant University, Km. 10 Idiroko Road, Canaanland,
P.M.B 1023, Ota, Nigeria
Tel: +234-1-7900724, 7901081, 7913282,7913283.
Website: www.covenantuniversity.edu.ng

Professor Kehinde O. Okonjo

Professor of Biophysical Chemistry,
Covenant University,
Canaanland, Ota.

Introduction

INTRODUCTION

CHEMISTRY: BETWEEN THEORY AND APPLICATION

1. The role of theory in science

It is a historical fact that man has been observing the natural world and recording his observations since ancient times. The oral communication of observations is even older. Observations such as the times and routes of migrating animals are of crucial importance to people who live by hunting; a knowledge of the rainy and dry seasons is essential to farmers. The importance of these and other natural phenomena made those whose knowledge of them was most extensive the leaders of their communities, and exceptional status was accorded to those who had, or were believed to have, the ability to predict such events. An excellent example of such a leader, and one of the earliest to be recorded, was Joseph (Genesis 41). We recall that Joseph, a foreigner and prisoner in Egypt, became the Prime Minister of that country because he was able to predict that there would be seven years of bountiful harvest followed by seven years of famine in Egypt and in the neighbouring lands. This enabled the Egyptians to save part of the harvest of the bountiful years for the years of famine.

Historically, prediction has been attempted (i) through an appeal to the supernatural or (ii) by means of a reasoned extrapolation of facts that were already known. These two approaches to the same problem are not as different as they might appear. If observed facts are believed to be under the direct and immediate control of God, then it is quite rational to consult Him about such events. This does not conflict with the making and recording of observations about such events. Thus, the ancient fascination with the prediction of the future led to an appeal to God but also to the recording and ordering of observations. The tendency to record and order observations was founded on the widespread belief that there must be a system or order in the universe. The challenge was to find this systemic order. To demonstrate that one has found it entails the ability to predict the results of observations yet to be made. This, the driving force of basic or fundamental science research, necessitates the collection of data and the arrangement of such data within some conceptual framework (or model) that makes them easier to understand, remember and use.

We can distinguish two broad categories of models. There are models of an essentially descriptive nature in which a phenomenon in question is likened to objects of our everyday experience. There are also mathematical models in which natural phenomena are described by a set of symbols, the meanings of which have to be defined, and which obey some particular rules of mathematical manipulation.

What do we mean when we speak of 'laws' in the physical sciences? What are these laws; how do they arise; and what is their value or purpose in science? The terms 'law', 'principle', 'theory' and 'hypothesis' as used in the natural sciences mean approximately the same thing. Any law, principle, theory or hypothesis that does not fit new experimental data must be amended. A physical law expresses, either in words or in algebraic form, the result which is to be expected of a particular experiment. Thus, Boyle's law may be expressed

(i) in words as, “At constant temperature the volume of a given mass of gas is inversely proportional to the applied pressure”; or

(ii) algebraically as, “$V \alpha 1/P$”, that is, $PV = c$, where c is a constant at any given temperature.

Once we have experimentally determined the value of the constant c for a particular gas, we can calculate either the volume V of the gas, given its pressure, or its pressure P, given its volume. For the so-called ideal gas the value of c is nRT, where n is the number of moles of the gas, R is the universal gas constant and T is the absolute temperature. Thus, the ideal gas law, arising from the *experiments* of Boyle and of Charles, is

$$PV = nRT.$$

It is important to emphasize that laws arise or are deduced as a result of experimental observation. It follows from this that they must also stand or fall by the results of any other experiment to which they relate. Thus the ideal gas law fails the test of application to all gases, especially in the region of low temperature and/or high pressure.

The value of laws to science and technology applies at various levels. A practical use of a law, which may be highly significant for applied science, is the prediction of a quantity which cannot be readily measured. An example is the necessity to calculate the gas pressure in a novel chemical plant which is still at the planning stage. A law also establishes a framework into which new experimental results may be fitted. It must be borne in mind that theory is a suggestion and is subordinate to the results of experiments.

2. Theory and application in chemistry: Le Chatelier's principle and the production of ammonia

2.1 The theory behind ammonia production

The reaction between hydrogen and nitrogen to produce ammonia is an equilibrium process:

$$N_2(g) + 3H_2(g) \qquad 2NH_3(g) \qquad \Delta H = -46\ kJ\ mol^{-1}$$

We shall use this reaction to illustrate the usefulness of Le Chatelier's principle (or law) in the industrial production of ammonia. Le Chatelier's principle may be stated as follows:

> *If a constraint is placed on an equilibrium mixture, then the equilibrium will shift so as to oppose the constraint.*

A manufacturer who is interested in making ammonia would want to get the maximum yield of his product. We observe that the reactants (N_2 and H_2) and the product (NH_3) are all gaseous. Gay-Lussac's law tells us that if we start with a combined volume of, say, four cubic metres of nitrogen and hydrogen in a ratio of 1:3, we end up with two cubic metres of ammonia. A constraint — a reduction in volume — has thus been imposed on the equilibrating system. According to Le Chatelier's principle, the equilibrium will shift to oppose this constraint, that is, it will shift to the left and very little ammonia will be produced. To increase the production of NH_3, pressure must be applied. Why? Because theory, here Boyle's law, tells us that if we increase the pressure on the reacting system its volume will decrease. Thus increasing the pressure increases the yield of ammonia. We also note that heat is produced as ammonia is formed: $\Delta H = - 46$ kJ per mole of ammonia produced. Thus, according to the theory (here Le Chatelier's principle), if we remove the heat produced by decreasing the temperature we should get a higher yield of ammonia. But here we meet a stumbling block! Our knowledge of kinetics tells us that as the temperature of a reacting system decreases, the *rate* of the reaction also *decreases*. So, although lowering the temperature should give a higher yield of ammonia, the *rate* of ammonia production would be so low that it would render the whole process useless to a manufacturer whose sole aim is to make a profit. In an industrial plant, a number of compromises have to be made: the reaction is typically carried out over iron catalysts at temperatures ranging between 400 and 600^{o}C and pressures from 200 to 400 atmospheres. These are the optimum conditions required for minimum production costs. Although the yield of ammonia could be increased by increasing the pressure above 400 atmospheres, the cost of production would be highly increased by such a further increase in pressure, which will require more expensive, specialized vessels that can withstand the additional pressure.

2.2 The economic importance of ammonia

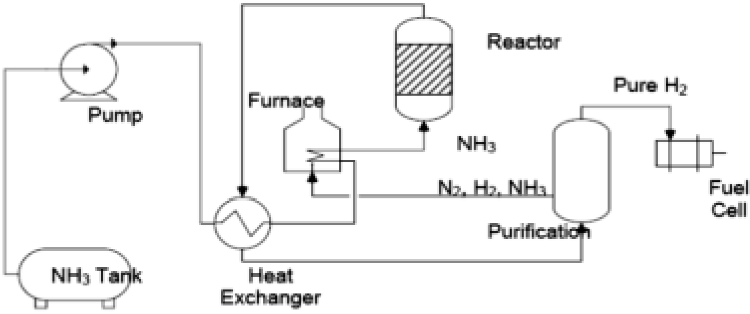
Ammonia is one of the most important industrial chemicals produced worldwide. It is used in the manufacture of fertilizers, nitric acid and polymers. Ammonia is normally produced by the catalytic reaction of hydrogen and nitrogen. The source of nitrogen is the air, but hydrogen is obtained from natural gas; other sources are petroleum coke or biomass. Although process technology has improved over the years, the basic chemistry is identical with the process developed by Haber and Bosch in the early 20th century. According to a US Geological Survey report, by 2002 the world production of ammonia was estimated at 131 million metric tons (1 metric ton = 1,000 kg). The importance of ammonia to the US economy is

seen from the fact that there is a good distribution network for it. There is currently a 4,950 km ammonia pipeline network in the US. These pipelines carry ammonia from central production sites to terminals serving distributors and end users, typically farmers. Other means of transportation are by ocean-going tankers, rail and trucks.

Map showing ammonia distribution network in the US

Why should Nigeria take an interest in the production of ammonia in the US and in other technologically advanced countries? Apart from the fact that Nigeria imports a lot of fertilizers for agricultural purposes, the major reason is that there are moves to transform the US economy into a hydrogen economy in which vehicles are fuelled by the reaction of hydrogen with oxygen in a fuel cell to produce electricity. In this way it is hoped to replace petrol with hydrogen in motor vehicles. A fuel cell is a primary cell in which the chemicals that produce electricity are constantly replaced as soon as they are used. By passing hydrogen and oxygen through a fuel cell, it is possible to generate electricity to drive motor vehicles and possibly trains. Some experimental cars have travelled at up to 80 km per hr. There are, however, disadvantages posed by using hydrogen directly, not the least of which is its tendency to explode in the presence of oxygen. Thus replacing petrol stations with “hydrogen stations” would pose explosion hazards for the ordinary motorist. Proposals have therefore been made to use ammonia as a carrier for on-board vehicular hydrogen storage. Ammonia, though, has its own problems. In particular, it has been declared a health hazard by the European Union. Therefore replacing petrol stations with “ammonia stations” will produce an environmental hazard. Moreover, although ammonia has a high capacity for hydrogen storage ─ 17.6 wt % based on its molecular structure ─ conversion to hydrogen will require that ammonia be cracked (see diagram below). Releasing hydrogen from ammonia in this way will require a significant energy input, as well as a significant reactor mass and volume. Fortunately for us petroleum exporters, the development of this technology has been put on hold because it will be highly uneconomical compared to the use of petrol, even in these times in which the cost of crude oil has climbed to almost $120 per barrel.

Conceptual ammonia processing system for hydrogen production



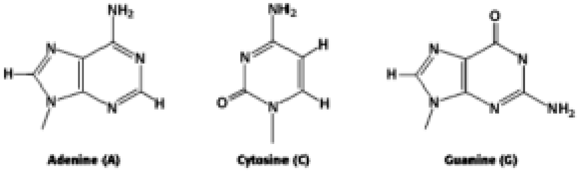
3. Theory and application in chemical biology: the genetic code and biotechnology

3.1 Mendel's 'traits' and genes

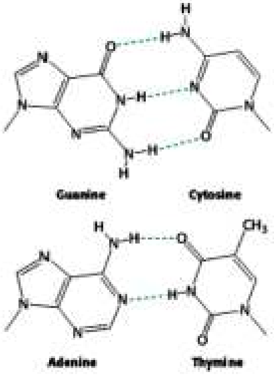
Farmers have known for centuries that the crossbreeding of animals and plants could produce certain desirable traits. Nevertheless, Gregor Mendel is considered to be the founder of modern genetics. Mendel's pea plant experiments conducted between 1856 and 1863 established many of the rules of heredity. Mendel had access to an experimental garden in which he could breed 'true' lines of pea plants and patiently wait for them to crossbreed in specified combinations. He worked with seven characteristics of pea plants, including seed colour. He demonstrated that when a yellow pea and a green pea were bred together their offspring plant was always yellow. However, in the next generation of plants, the green peas appeared in a ratio of 1:3. He concluded that green peas were 'recessive' and yellow peas 'dominant'. He thus demonstrated the effect of invisible 'factors' — what we now call genes — in providing visible traits in predictable ways. Mendel's experiments are a beautiful demonstration of basic or fundamental research at its best. It is probably safe to state that before the advent of Gregor Mendel the science of biology was merely an observational discipline lacking the strong theoretical platforms of chemistry and physics. With Mendel's laws of heredity, biology had for the first time a potential theoretical basis of its own.

The first result identifying deoxyribonucleic acid (DNA) as the carrier of genetic information was published in 1944 by Oswald Avery and his colleagues. They demonstrated that genetic information was not carried by proteins, as was thought, but by the nucleic acid, DNA. With this discovery, many scientists shifted their attention to a study of nucleic acids. The most successful of these studies was conducted by Erwin Chargaff, who found that the DNA composition differed from one species to another. He also found that the nitrogenous bases adenine (A) and thymine (T) appeared in the DNA of different species in equal amounts; so did guanine (G) and cytosine ©.

Structures of adenine, cytosine, guanine and thymine



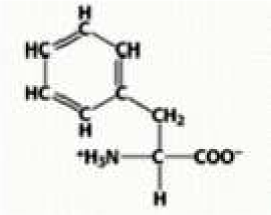
This finding later proved to be important for determining the x-ray structure of DNA. By the early 1950s, it was known that DNA was composed of sugars, phosphate groups and equally matched nitrogenous bases. The x-ray crystallographic data of Maurice Wilkins and Rosalind Franklin enabled James Watson and Francis Crick to solve the double helical structure of DNA. In this structure adenine is joined to thymine by two hydrogen bonds and guanine is joined to cytosine by three hydrogen bonds. The mode of combination of these base pairs is shown in the diagram below.



Proteins are the molecules that perform most of the functions in the body. They are made up of many amino acids joined together by peptide bonds. How does the genetic information in DNA get translated into proteins? In other words, what is the genetic code, that is, how many bases code for an amino acid? Since four nitrogenous bases appear in DNA, a two-letter code would give rise to 4^2 code words, that is, 16 amino acids. There are 20 naturally occurring amino acids in proteins. Consequently, a two-letter code would not suffice. A three-letter code would give 4^3 code words, i.e., 64, a number that is sufficient to account for the 20 amino acids found in proteins. This large number also indicated that the code was degenerate and that an amino acid could be coded for by more than one three-letter code word.

The next step was to identify the code word for each of the 20 amino acids. The first breakthrough in this search came in 1961. Using the cytoplasm of E-coli cells in a cell-free system, together with synthetic polyuracil (poly-U) as mRNA, the group of Marshall Nirenberg identified the three-letter code UUU as the code word for the amino acid phenylalanine:

Structure of phenylalanine



Subsequent work by others, including the Indian synthetic chemist Har Gobind Khorana, helped to establish the complete genetic code.

The genetic code

First position (5′ end)	Second position				Third position (3′ end)
	U	C	A	G	
U	Phe	Ser	Tyr	Cys	U
	Phe	Ser	Tyr	Cys	C
	Leu	Ser	Stop	Stop	A
	Leu	Ser	Stop	Trp	G
C	Leu	Pro	His	Arg	U
	Leu	Pro	His	Arg	C
	Leu	Pro	Gln	Arg	A
	Leu	Pro	Gln	Arg	G
A	Ile	Thr	Asn	Ser	U
	Ile	Thr	Asn	Ser	C
	Ile	Thr	Lys	Arg	A
	Met	Thr	Lys	Arg	G
G	Val	Ala	Asp	Gly	U
	Val	Ala	Asp	Gly	C
	Val	Ala	Glu	Gly	A
	Val	Ala	Glu	Gly	G

3.2 From the genetic code to biotechnology

Biotechnology arose from the development of recombinant DNA technology in the early 1970s by Paul Berg, Herbert Boyer and Stanley Cohen. This technique made possible the combination of genetic material from unrelated species. The combined genetic material could be amplified to relatively large quantities in a suitable host, such as the bacterium *E. coli*. This paved the way for the development of recombinant proteins. For example, insulin can be produced in relatively large quantities using recombinant DNA technology. Those who suffer from type 1 *diabetes mellitus* do so because their bodies do not make sufficient insulin to utilize carbohydrates. This leads to the uncontrolled breakdown of lipids and proteins. The net effect is that the kidneys eventually become overwhelmed. The production of large quantities of insulin through recombinant DNA technology means that type 1 diabetes can be treated with relative ease.

Sickle cell anaemia is a black man's disease affecting a sizeable percentage of the population. It arises from the single mutation $\mathrm{A3[6]}\beta^{\mathrm{Glu}\rightarrow\ \mathrm{Val}}$ in each of the β chains of sickle cell haemoglobin relative to normal human haemoglobin. This mutation represents a change of 0.35 % (2 out of the 574 amino acids in the haemoglobin molecule); and yet the unfavourable physiological consequences are far reaching. It is hoped that with the success of the Human Genome Project this molecular disease will one day be cured through recombinant DNA technology.

4. The value of basic research

Basic research (also known as fundamental or pure research) is research that is driven by a scientist's curiosity or interest in a scientific question. The major motivation is not immediate application for commercial gain but to expand the frontiers of knowledge. Most scientists believe that a basic, fundamental understanding of all branches of science is required for progress to be made. We have shown above how the basic research conducted by Boyle, Charles and others has made a positive contribution to progress in optimizing the conditions for the production of ammonia. We have also shown how Gregor Mendel's pea plant research has spun today's biotechnology industry. There are other historical examples in which basic research has played a vital role in the advancement of scientific knowledge. Many of today's electrical devices (e.g. radios, alternators and generators) can trace their roots to the basic research conducted by Michael Faraday in the 1830s, during which he discovered the principle of electromagnetic induction, that is, the relationship between electricity and magnetism.

Today's civilization is totally dependent on electricity. Our understanding of the properties of x-rays began with the fundamental research of Wilhelm Röntgen in the 1890s. Today, x-rays are used in medical diagnosis, in the determination of molecular structure, and in numerous other ways that are beneficial to man.

What is the attitude towards basic research in the advanced countries?

The following resolution passed in 2004 by the Council of the European Union immediately attracts attention and speaks volumes on the attitude of Europeans towards basic research:

"The Council acknowledges that the main objective of high quality basic research is the development and enhancement of knowledge, thereby contributing to the advancement of science and to promoting sustainable economic development, competitiveness and employment in the knowledge based economy; acknowledges also the positive impact that high quality basic research will have on society as a whole; reaffirms therefore the importance of reinforcing support, also with the involvement of the private sector, for basic research in the context of the European Research and Innovation Area; welcomes the fact that the Commission, in its communication 'Europe and basic research', examines the impact of basic research in the competitiveness, growth and quality of life in Europe and puts forward suggestions for exploring the means of strengthening Europe's performance in basic research; recognizes the need to:

-continue to work to improve the climate for the development of science and research careers in Europe and the key role of basic research in training researchers;

-stimulate research excellence of world class quality in Europe in a wide range of sectors and disciplines, including social sciences

And humanities, by encouraging more competition in science-driven research at European level selected on the basis of excellence;

-improve the exploitation of results of basic research by supporting transfer of knowledge between researchers, centres of excellence and enterprises, with particular reference to the role of universities, as well as within society as a whole; …..”

5. Stemming the brain drain from Nigerian universities

We have had a brain drain from Nigeria to the United States and Europe. More recently there has been a brain drain to Southern African countries, especially to the Republic of South Africa. In addition to these, we have an internal brain drain from the universities to the business institutions. Unless the governing authorities in Nigeria recognize that Nigeria has a problem — a very serious one at that — the country might be headed for an educational and economic eclipse. Recognizing that there is a problem is one thing; doing something about it is another. The government should follow the example of Europe and recognize the importance of funding higher education at the postgraduate level where basic research is done. The future economic and social advantages of the increased high level human capital stemming from such an investment can only be imagined.

The good news is that there is hope for Nigeria. By establishing Covenant University with a vision that is radically different from those of the older universities, namely, to train a new generation of leaders who have imbibed a set of life-transforming core values, the founders have made a departure from the norm. The success of this new vision is now evident for all to see. It is my earnest hope and prayer that those who wield political power in this country will not only see but also emulate the excellent example of Covenant University.

6. Conclusion

Basic research is the least expensive form of research and is affordable to governments with only modest resources. Although it does not bring about immediate economic results, it creates a very solid base for economic and social development. It is the job of basic researchers to inform, advise and warn society in general and those who hold political power about the dangers of neglecting this sector of the economy. Any country that wishes to be more than just an amusement park or a source of cheap labour must build and cultivate a solid higher education base, especially at the postgraduate level. This is inseparably linked with quality basic research. Perhaps a good model to copy would be the National Research Foundation established in 1999 in South Africa to "support and promote research funding, human resource development and the provision of necessary research facilities, in order to facilitate the creation of knowledge, innovation and development in all fields of the natural and social sciences, humanities and technology…"

7. Acknowledgements

I wish to express my sincere gratitude to my wife, Mrs. Chinwe Okonjo Adigwe, a retired Chief Executive of the University of Ibadan Publishing House, for editing the text of this lecture and ensuring that errors are eliminated as much as possible.

I thank the Almighty God, our Father, for the vision He gave to our Chancellor, Dr. David Oyedepo, which led to the founding of Covenant University, this great citadel of learning. I feel highly honoured to have been selected by the Vice-Chancellor, Prof. Aize Obayan, to give the first public lecture for the 2008/2009 academic year. This month, September, is the month in which our Chancellor celebrates his birthday ─ to be exact, on the 27th. I had wished to give this lecture next February, the month in which my wife celebrates her birthday, so as to dedicate it to her; but my wife is delighted to have me dedicate the lecture to our Chancellor. It is, therefore, with great pleasure that I dedicate it to the Chancellor, Dr. David Oyedepo, a man of vision, a firm believer in education, a strong advocate of research, and a committed provider of research funding.

To all our guests I say, "Thank you very much for coming and for listening very patiently." May the Lord bless you all! Amen.

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