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Chemistry: the great ideas*

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Abstract: What are the central ideas of chemistry that we should ensure that our students carry with them as they travel through an educational system and out into the world? Indeed, what are the great ideas that give a chemist's vision of the world such a distinctive character, and which we would wish the general public to comprehend? Chemistry is such a central science for both our students and our communities that we should ensure that we do not dissuade our students and our public from discovering the insights it provides. In this talk I shall endeavour to identify first the difficulties of teaching our subject, then the dozen or so great ideas that, in my view, should be the spine of our courses. I will examine the general principles that make chemistry such a central part of any scientific education and in particular a component of the physical sciences. Then I shall identify the individual topics that I regard as the foundations of chemistry. The latter I shall do at three levels: at freshman level, for those who need to be aware of chemistry but not in great depth, to those in physical chemistry, who do need a deep understanding of our remarkable subject, and to the general public, who should be aware of a subset, at least, of our ideas.

What are the principal concepts of chemistry that we should teach to our students? I shall concentrate on introductory chemistry in this talk, and try to identify the concepts that we chemists should hope our students will carry away from our courses into their careers, whatever these careers may be. At the same time I will be directing my remarks at instructors who are devising courses to introduce chemistry to students. I shall also have in mind one of the most important of our tasks: the communication of our remarkable subject to that most suspicious and unwelcoming audience, the general public.

First, I would like to share my general attitude to education in chemistry. The principal target of our education should be to find a way to bridge the imagined to the perceived. By that, I mean, we should show people how to look at a lump of matter, and in their mind's eye, see it as a collection of atoms and molecules. Then we should teach them to judge between conflicting influences. That is the essence of our subject, for it is rare that a single property governs the outcome of a reaction. We need to train our students to judge the likely outcome of conflict. Third, we need to show how to express qualitative ideas quantitatively. That ability brings chemistry into the domain of the physical sciences and puts the enormous power of mathematics into our hands.

But what is it that makes our subject so difficult? One feature, which I have already touched on, is that chemistry is the science of conflict. The problem of knowing whether it is electronegativity, hardness, or some other property that is governing a physical or chemical property undermines confidence and makes our subject seem difficult to penetrate, let alone master. Second, ours is an intricate subject, and it is very difficult for people to master sufficient detail to give themselves confidence to make rationalizations, let alone predictions. The third difficulty is that, despite our subject being the most tangible of all it is also highly abstract. Our currency of discourse seems to the general public at least, highly abstract. As soon a chemists start to speak, out tumble all manner of abstractions, such as atoms, molecules, energy, entropy,

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and so on. We know that our principal concepts are not abstractions, and a part of the battle is to render our concepts so that they seem real.

So, with those thoughts behind us, let us turn to our principal concepts: what are the great ideas of chemistry? at this point, I do not want to promise too much. These are fundamental ideas, and as such are necessarily simple ideas that everyone already knows. These are the ideas that, in my view underpin and mark out our subject.

1 *Matter consists of about 100 elements.* It is a wonderful achievement of chemistry that it has shown that the world is a composition of so few entities. Of course. physicists have gone further, and have reduced the world to far fewer fundamental entities, but at 100 fundamental entities the entities retain their personalities and hence give chemistry its richness.

2 *Elements are composed of atoms.* The atom is the fundamental unit of our currency of discourse. and is the foundation not only of our understanding of chemical properties but also of the manipulations of chemistry and stoichiometry. Here Lavoisier is the particular god from whom this concept ultimately springs, for he first brought the chemical balance to bear on chemistry and achieved the extraordinary feat of attaching numbers to matter.

3 *The orbital structure of atoms accounts for their periodicity.* The periodic table is, of course, the icon of our subject, and it is extraordinary that it can be explained in terms of a few simple ideas about orbitals, their energies, and the Pauli principle. It is remarkable that so much that can be rationalized by so little.

4 *Chemical bonds form when electrons pair.* Another god of chemistry is G. N. Lewis, who among his many achievements had the insight to identify the electron pair as the central content of the chemical bond. It is all the more remarkable that he did so before the ideas of quantum mechanics had been fully formulated, We know that there are exceptions to Lewis's approach, but his simple, central concept carries us far into chemistry.

5 *Shape is central to function.* We all know that it is simple ideas, such as the atomic radii of the element and related properties that determines, to a large extent, the bonding characteristics of the element, and how the shapes of molecules, particularly of enzymes, determine their properties. Incidentally, once the general public understands that chemistry's abstractions are in fact tangible, they should feel more comfortable with our so-called abstractions.

6 *Molecules attract and repel each other.* At this point we encounter the all-important bridge that takes us from the world of atoms (in a sense, the word of the imagined) to the world of bulk matter (in a sense, the world of the perceived). To make the connection, we need to be able to translate the properties of individual entities into emergent properties, and for that we need intermolecular forces.

7 *Energy is blind to its mode of storage.* Related to the bridge from atoms to the bulk, we have the foundations of statistical thermodynamics. The Boltzmann distribution is probably the most profound concept in chemistry. It is ostensibly a highly determined structure (the exponential decline of population with increasing energy) but its derivation shows that it is based on complete randomness; the distribution of populations over the available states with equal *a priori* probabilities. Then, with the structure established, we have an expression of enormous power, particularly for establishing the properties of bulk matter. Moreover, the distribution neatly captures the spirit of chemistry. Most of the population lies at low energy levels: and hence we have an understanding of why most matter survives for long periods. Yet the distribution also has a tail at high energies. So it also allows for the possibility of change from one structure into another. Indeed, if I were participating in a 'balloon debate' (in which each participant as argue that he should not be thrown out of a sinking balloon), then I would feel very comfortable arguing on behalf of Boltzmann and his distribution.

8 *Reactions fall into a small number of types.* We are all familiar with the classification of reactions into proton transfer (Brønsted acid–base), electron transfer (redox), and electron-pair sharing (Lewis acid–base). Here we encounter the second great simplification, in which we see not only that all matter can be reduced to 100 or so elements, but that the transformations of matter can be expressed in terms of about three types of process. Here we see part of the nobility of the scientific attitude, the reduction of the complex into concatenations of simple entities.

9 *Reaction rates are summarized by rate laws.* One of the techniques that physicists are very good at is building differential equations to summarize phenomena, and then extracting the juice of their solutions. We chemists are not nearly as good at this technique, but we are becoming good at it in one very special region, that of rate laws. Rate laws provide a window on to mechanism. However, until recently, all chemists have been able to do is to trivialize their rate laws and have found solutions that have very little content. Now, though, with the aid of computers, we can solve the highly nonlinear differential equations that result in periodicity. At last, the patterns of nature have come within chemistry's grasp.

At this point I would like to indulge in the luxury of talking more explicitly about physical chemistry. Of course, almost all I have said already can rightfully be considered as lying within this domain, but I would like to focus here on the *equations* of physical chemistry. What are the most important equations?

I can identify a small handful of absolutely crucial equations. One obvious one is the Schrödinger equation:

$$H\Psi = i\hbar\dot{\Psi}$$

That is an obvious one to mention, but notice that I have written the time-dependent form of the equation, as it is so much richer than the time-independent equation, capturing as it does the whole of spectroscopy. Then, for the central equations of thermodynamics I think I would like to select two relations involving the Gibbs energy:

$$\Delta_r G^\circ = -RT \ln K$$

which links the whole of thermodynamic data to the conditions relating to equilibrium, and

$$\Delta G = w_e$$

which links the Gibbs energy to electrochemistry. For my final selection of this very sinewy crew, I choose the Boltzmann distribution:

$$\frac{N_i}{N} = \frac{e^{-E_i/kT}}{q} \qquad q = \sum_i e^{-E_i/kT}$$

I have already explained why this expression is so central. These, I think, are the stepping-stone equations of physical chemistry. Our students complain that physical chemistry is so mathematical: but if they knew that this is all that truly matters, they would be content!

Let me conclude. I consider that it is essential that we instill a sense of insight into our students, and let that developing insight guide their gradual acquisition of the more recondite parts of our subject. We should not try to teach them everything—it is more important to teach them to be lifelong acquirers of knowledge than to turn off their love of the subject by overburdening them with information at the beginning. Above all, we should cultivate a love of this centrally important sciences, and endeavour to show people—young and old—the beauty of this glorious world as seen through a chemist's eyes.