Case Study Exchange Format – HIPST
Chemical Paper Tools (Modelling)

Details of section	Guidance
1. Title	Chemical formulae and equations: more than just calculations? Key words: formulae, equations, modelling.
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3. Abstract	The activity is relevant to upper secondary school science, and for all abilities. We advocate a fresh approach to chemical formulae that widens the focus from algorithmic balancing equations and routine calculations. We recommend one that focuses on the endeavours of chemists from the past to lay the quantitative foundations of chemical materials and reactions through the processes of painstaking and careful analytical chemistry, and that recognises the character of formulae and equations as meaningful representations of fundamental chemical processes. We adopt a semiotic (semiotics: the study of signs and symbols, especially as means of language or communication) approach that focuses on the meanings of the components and of the whole of the formulae and equation. To do this, we need to examine the creation of conventions of chemical symbolism, and the role of chemists who made these conventions in history. We also examine ontology, or nature, of the entities that make up formulae and equations. In the case of formulae, the nature of the entities is often implicit, so that whether particles are ions or molecules is often hidden in some formulae. We discuss why there are discrete molecules in some materials but none in others that have a giant structure, for example. In the case of equations, we imagine the value of word equations, against symbolic equations. There is a range of equation types rarely discussed at this level, but whose richness of meaning helps us to delve into the meaning of the chemical processes themselves. We do not lose sight of the calculations altogether, since they represent a secondary importance of the equations, but rather adopt a critical stance that sees calculations as applying to ideal situations, but not quite real life where the equations only approximate to the concrete position.

	The outcomes are more than a deeper understanding of formulae and equations themselves, but a more general view of the significance of conventions and symbolism in this part of chemistry. A sceptical approach to realism is also an important aim of this topic.
4. Context	The Case Study Introducing HPS in the school chemistry curriculum is a relatively recent activity for curriculum designers and researchers, compared with physics. There are significant reasons for this. 1. There are few recognised paradigm changes in chemistry compared, for example, with physics. The usual ones quoted include the phlogiston idea, although this only lasted for 50 years in history, and quantum mechanics, which is, perhaps, more properly located in physics. 2. There are few historical artefacts that have lasted in chemistry, compared with physics which has abundant examples. Partly this is because chemistry widely used glass apparatus which is fragile and easily destroyed. Partly it is because some of the equipment, such as the balance, were considered to be so common-place that they were simply not worth saving or recording. Partly it is because the furnaces that were used were destroyed. Finally, partly it is because many of the early chemical discoveries were based on phenomena, and not on measuring instruments. 3. The structure of the chemistry curriculum in schools is such that phenomenological investigations abound at junior levels, and quantitative considerations, such as calculations based on chemical formulae and chemical equations are treated and assessed in an algorithmic way. This Case Study arises from two sources. The first is a personal frustration at the low level challenge in the present science curricula on chemical formulae and chemical equations. ‘They represent common compounds by chemical formulae and use these formulae to form balanced symbol equations for reactions.’ (QCDA 2007) The requirement is for balancing equations and for simple mass calculations based on balanced equations. This is hardly challenging and treats these two topics in an algorithmic sense. The second is a book on *Experiments, Models, Paper Tools: Cultures of Organic Chemistry in the Nineteenth Century* by Ursula Klein in Berlin. She analysed the use of chemical formulae by organic chemists in the 19th century as they battled to understand the chemical processes. ‘A central argument of the book is that chemists began applying chemical formulas not because they believed in the truth of disembodied theory, and not as a passive medium for expressing and illustrating extant knowledge, but rather as productive tools on paper or "paper tools" for achieving new goals. The notion of "paper tools" highlights nineteenth-century chemists' pragmatism towards high-level theories and their use of such theories in practice for conducting experimental research and for classification. It further serves to focus historical analysis and reconstruction on the semiotic, material and performative aspects of representation, model building and conceptual development. Paper tools share many features with laboratory tools and performances, without being

> identical to them. They are material devices in a semiotic sense, that is, they are visible and manoeuvrable marks on paper. Their manipulation is guided and constrained by their syntax and social rules of application, rather than being performed at will, just as the practical application of a physical tool is guided and constrained by technical design and collectively shared skills.' (From a book summary on the web site of the Max Planck Institute for the History of Science)

This book has inspired this topic to explore a richer side of chemical formulae and chemical equations, that of semiotic tools that can reveal chemical insight. As with all the HIPST modules, a great challenge has been how to construct a module on History and Philosophy of Science that is authentic in its interpretation to the original context, while being simple enough to be accepted by the target group of learners.

The topic begins with the idea of conservation of mass in chemical reactions, implicit in the focus on balancing equations. It would seem to be obvious that mass is conserved once an atomic understanding is adopted but to show this experimentally was a significant challenge. It involved a step up in the sensitivity of the common balance, no mean feat for Lavoisier who first tackled this problem. He relied on a great instrument manufacturer, Fortin, using very sharp balance pivots and long, rigid, balance arms. Lavoisier also used his previous experience as an accountant to set up his mass balance sheets, in the form of an account ledger. Many reactions are difficult to contain if they involve gases, or to control for changes in mass if they heat up too much, so Lavoisier was limited to only a few reactions. So, what did he find? In some cases, mass was not conserved. Lavoisier should have abandoned his ideas but he was so convinced that he put his failures down to experimental error, including some that he could not find. It was left to Landolt later to make further investigations but he found the same, that in some cases mass was not conserved. Even a much more careful and recent investigation in the 1950s failed to find evidence that mass was always conserved. Nevertheless, we maintain the idea that mass should be conserved., in spite of the evidence.

The next step is to examine how to determine formulae, and the first part of this is the Law of Constant Composition. Exercises in determining percentage mass composition were common in the middle third of 20th century chemistry in schools, and, indeed, were used to assess practical prowess of students. These days, such determinations are all but extinct. They were the mainstay of chemical progress in the 19th century. The Law of Constant Composition is a vindication of atomic theory, since it is difficult to see how it could not be if the atomic theory was valid.

Determination of empirical formulae from mass composition is a routine calculation. However, the determination of molecular formulae is not so easy, as the Chemists at the Karlsruhe Conference in 1860 discovered. The idea of a molecule was not that obvious.

	Chemical formulae have their own conventions, often based on historical decisions by the chemical community. There is a range of chemical formulae, with their own conventions, and within them, a range of depictions of bonds and electronic structure. Mining these formulae for meaning is a worthwhile educational task in itself, much of it related to the history of symbolism development. Having determined formulae, the task now is to find out the ratio of reacting molecules, to construct a chemical equation. Various web sites claim to have workable paper-based algorithms for balancing equations. We feel it is important to construct them from empirical data, as a connection to the real world. The semiotics of chemical equations is rich territory to be explored to promote students' understanding of chemistry at the symbolic level. There is a range of chemical equations, with their own conventions, and within them, a range of arrows and commentary terms, such as added heat. Mining these equations for meaning is a worthwhile task in itself, much of it related to the history of symbolism development. The story goes on for chemistry but it stops here for this module. We intend to have the students explore meaning, and in so doing, bridge the old gap between the macroscopic, sub-microscopic, and symbolic forms of representation.
5. Topic and curricular relevance	The target group in England is able 15-16 year old students, in schools. The scientific concepts and processes include: *Concepts* • Law of Conservation of Mass • Law of Constant Composition and its relation to atomic theory • Chemical formulae determination. • Chemical equation determination *Processes* • Establishing analytical techniques *History of science* • Conventions for symbolism in formulae and equations • Law of Conservation of Mass • Law of Constant Composition • Development of Atomic Theory *Nature of Science* • Semiotics of formulae representation • Semiotics of equation representation

	Expected outcomes of learning See above. *Links to formal science content* ‘They trace the development of science worldwide and recognise its cultural significance.’ (QCDA, 2007, England National Curriculum) The GCSE (16+) syllabuses mention formulae, equations and calculations but with no details. The new National Curriculum (2007) in England has no direct references to History and Philosophy of Science ideas, and textbooks rarely refer to history of chemistry except for brief biographical notes on some memorable scientists. Development of science is almost always in terms of contemporary science. Philosophy of science, as in scientific method, is a limited view position based on Popperian logic of testing theories with data in a positivist way. *Expected effects on student interest and motivation* • Expected that students would be excited by spectacular practical work. • Expected that students would be engaged in reflection activity. *Expected learning of general scientific skills such as communication, socio-scientific decision-making, and collaborative learning.* • Yet to be explored
6. Historical background	Examples of quantitative analysis or synthesis of compounds go back to at least the seventeenth century according to Partington in his A Short history of Chemistry (Dover Publications, 1957, 3rd Edition) with a description of Kunckel (d.

7. Social, political, and cultural background to history	1703) weighing of the formation of silver chloride. Bergman (d. 1784) made a large number of analyses of metal salts. These determinations seemed to have established the Law of Constant Composition, or at least were dependent on that Law being true. Proust (1754 – 1826) made a long series of quantitative investigations before his laboratory was pillaged by the French army in 1808. Proust is credited with stating the Law of Constant Proportions in 1799 and 1806. Sadly, the histories do not describe the balances that must have been used. Although signs of the atomic theory had been independently proposed, it took a long time for chemists to link the constancy of composition to this theory through the notion of fixed atomic weights. T is not clear from the histories how this link actually formed. The historical time of these events was full of revolutions and military coups, as shown in the French Terror of the late eighteenth century, incorporating the beheading of Lavoisier at the guillotine. Social links were important for chemists, not least in staying alive for some of them. Strangely, the idea of a chemical reaction being an example of the conservation of mass was widely accepted without accurate testing. We may never know, but the relative insensitivity of balances may have precluded a serious investigation until Landolt working from around the turn of the 20th century reported some systematic deviation from the Law of Conservation of Mass. This has been confirmed by Volkammer and Streicher working in parallel but separately in Germany and the USA in the 1950s. they could not reasonably explain their results. However, chemists carry on ignoring this evidence and assume that the mass does not change. Establishing formulae from such quantitative work continued apace until, by the early nineteenth century, most formulae had been well determined (apart from some famous aberrations such as HO for water). This contrasts with the present algorithmic determination of formulae of metal salts from ionic charges, assuming neutrality of the final compound, with no reference to practical determinations. Organic chemicals are rarely amenable to such routines for the age range 11-16, and formulae have to be remembered. The origin of chemical equations is also a little uncertain. Liebig (in Traité de chimie organique, 1840-44) uses equations sparingly, according to Partington, while Gmelin uses them freely in his Handbook (1848-72, English translation).

8. Philosophical background, including the Nature of Science	The traditional use of chemical formulae and equations conveniently ignores philosophical considerations. However, there are two philosophical considerations to be explored. The first is the link between formulae and atomic theory. We can imagine that experimental evidence for constant composition gave rise to atomic theory but there is no evidence for this. It seems that it was fortunate that the atomic theory, with its fixed mass atoms, was around to explain the Law of Constant Composition. Certainly, the atomic theory provided a strong imperative to believe in the Law of Conservation of Mass, when there was no effective way of testing it, and to stick to the Law even when the evidence (Landolt) was against it. The second is the vexed place of chemical equations in chemistry, resulting in the strong focus on balancing, based on the Law of Conservation of Mass. We now know that many reactions can go alternative ways, so that we can not assume that only one equation is involved. Incomplete combustion is but one example but they abound in organic chemistry. Yet again, the focus is on simplification, when it can only lead down a cul-de-sac.
9. Obstacles to teaching and learning	There has been some research about differences between chemical and physical change, perhaps because chemistry is littered with dichotomies at the early stages, based on macroscopic behaviour, yet it is clear that the difference only makes sense at the sub-microscopic and symbolic levels. These levels are beyond the pupils in the early stages. Chemical formulae and equations are introduced as symbolic representations without focusing on different ways of representing first. This module intends to set this straight. The lack of accurate equipment for weighing, and appropriate skills for carrying out the weighing competently, are major barriers to progress.
10. Methods and media for learning	Practical work is central to this topic, although some of the evidence must come from secondary sources from the last point in 9 above. Newspapers are employed for informing about historical and philosophical matters. Some YouTube video material is also available.
11. Pedagogical skills	Yet to be explored
12. Research evidence	Yet to be explored
13. Author's reflections	There were a number of factors that influenced the study. Some of these were inevitable and out of control of the researcher, while others could be changed. • In the middle of the project, for personal reasons, the researcher was unable to meet with teachers for a considerable time to design the Case Studies. This led to delays in design but also to a method where the researcher provided an overall structure that was then modified during trials. Since the teachers had expressed their view that their personal knowledge of HPS was limited, this provided a base for their work, such that the teachers saw this as a strong learning activity for them. In the first place, they claimed that they would simply enact the strategy in their classes but it was clear that local circumstances and their personality led them to adapt the programme.

14. Further user professional development	This is well provided in the associated wiki-site at www.ukhipstmodelling.wikispaces.com
15. Written resources	*A copy of each of the written resources should be provided as an appendix*

Appendices

Modelling through chemical equations – topic overview

Topic	HPS	Comments
Introduction to modelling at macroscopic and sub-microscopic levels: pressure in syringes (see PALAVA experiment below) The PALAVA project - a method of assessing modelling capability The survey work is well described in this article.	**History:** Article on The Era of Alchemy by Greg Goebel, in the public domain; do read the section on The Rise of Scientific Ideas for comments about the challenges of studying gases when they can not be contained. The article suggests that 'the long-lost atomic ideas of Democritus, who had correctly envisioned air as particles bouncing around in a vacuum' 'had resurfaced in the 15th century, and made a convert in the form of the French philosopher Pierre Gassendi (1592:1655), who spread the word'. A biography of Democritus is in Wikipedia Another biography of Democritus (Stanford Encyclopedia of Philosophy). Whether Democritus understood a vacuum (void) in the same way that we do now is debatable. Both Boyle and Toricelli in the 17th century created models of air based on quantitative data about air, e.g. the effect of pressure on air volume at a fixed temperature. Bernoulli developed these in 1738. **Philosophy** Democritus' views on epistemology, and whether senses can discover truth are discussed in the Wikipedia biography . This is further discussed in the Stanford text. The Stanford text contains an excellent discussion of ancient Greek philosophy in a reasonably accessible tone, for teachers. The ideas of the Greeks came from thinking, i.e. philosophy, not empirical and practical investigation. A Wikipedia biography of Pierre Gassendi is available but is tough	**Avoidance of whiggishness:** Looking at whether Democritus' ideas about a void and atoms are the same as today. **Learner material:** Biography of Democritus Biography of Toricelli **Teacher material (other than that provided for learners):**

	reading, in line with the ideas of the time!	
Clues about compounds: law of constant composition as an indicator of atoms Clues about law of conservation of mass: efforts to represent atoms.Third level of representation i.e. symbolic. Issues about balancing equations. Practical on formula of magnesium oxide here.	**History**: Law of constant composition (definite proportions) from Wikipedia here See pictures of balances from Science and Society picture library here. Note Ramsden's balance from late 18th century, and the 'self-indicating balances designed by Da Vinci, 1452-1519'. Lavoisier computed masses, using an accountant's expertise (he did work as in the *Ferme Generale* collecting taxes for the French government, for which he was beheaded in 1794 on the guillotine) and his tables (reproduced here) look very similar to financial tables. 'The oldest surviving balance used for a published series of chemical experiments is said to be that used by ... Joseph Black', described in his doctoral thesis of 1754 (quoted here). Black's balance had a sensitivity of about 1 in 14000) Jon Berzelius' fundamental work is written in Wikipedia, including his symbolic forms that represent elements and atoms. Chemical Heritage Foundation on Lavoisier here **Philosophy**: Induction is the process by which ideas about atoms were proposed to explain constant composition of compounds. Explanation from Intute web site Given incompleteness of chemical reactions, can equations be balanced? A major problem in traditional quantitative analytical chemistry was to ensure firstly that the materials used were pure, and secondly, that the reaction used for calculations proceeded 100% as written.	**Avoidance of whiggishness:** From Wikipedia - ' The law of definite proportions might seem obvious to the modern chemist, inherent in the very definition of a chemical compound. At the end of the 18th century, however, when the concept of a chemical compound had not yet been fully developed, the law was novel. In fact, when first proposed, it was a controversial statement and was opposed by other chemists, most notably Proust's fellow Frenchman Claude Louis Berthollet, who argued that the elements could combine in any proportion.The very existence of this debate underscores that at the time, the distinction between pure chemical compounds and mixtures had not yet been fully developed. This part of chemistry marked progress in manufacture of chemical balances (see here) (Lavoisier had his balances made in the Netherlands by Nicolas Fortin (biography here)and Pierre Bernard Megnie) **Learner material:** Law of constant composition Nature of philosophical induction Chemical Heritage practical on fermentation here. It is aimed at early undergraduate level. Chemical Heritage practical on magnesium

		burning here. A Chemical Heritage paper on Lavoisier's instruments as Objet's D'Art is here. **Teacher material (other than that provided for learners):** Non-stoichiometric compounds from Wikipedia
Chemical change and its representation in equations. Chemical equations v mathematical equations Practicals on chemical equations, such as iron and copper(II) sulphate in solution.	**History** First chemical equation (1615) by Beguin here Biography of Cullen (1710-1790) (used diagrams as chemical equations) here Biography of Lemery (1645-1715) here. **Philosophy** Nature of representation Stanford - Mental Representation Nature of scientific modelling What is the nature of the distinction between chemical and physical change? Is it helpful, powerful or simply plain wrong? Some of the history of its introduction may be a good start.	**Avoidance of whiggishness:** Development of systems of chemical representation took place over a long period of time. The challenge was to infer sub-microscopic explanations from macroscopic phenomena. **Learner material:** Beguin and Cullen's early attempts to write chemical equations. John Dalton's symbols (see Wikipedia here) **Teacher material (other than that provided for learners):** Mental modelling
Signs in chemical equations; origin and use	**History** History of + sign in chemical equations History of chemical arrows Braille chemical signs and symbols **Philosophy** Semiotics for beginners - nature of signs	**Avoidance of whiggishness:** The impact of external influences such as printing technology on conventions for printing chemical equations demonstrates the complex interchange between the rationality of chemists making decisions about their discipline and others. **Learner material:** History of signs in chemical equations, focusing on + and = signs, as opposed to arrows, based on Oversby papers.

		Teacher material (other than that provided for learners): Semiotics for beginners - nature of signs All of the web sites visited on 2 Dec 08, by Googling Chemical Notation, focused only on expressions of formuae, and not on the signs, such as arrows, and +. The Braille site is mainly concerned with arrows. there are many computer sites concerned with mark up of chemical formulae but not signs. **Avoidance of whiggishness:** This topic is modern and whiggishness is not a problem.
Computer animations of chemical processes - a step in representation	**History** First of an article on the history of animating is here. Wikipedia full article on history of animation **Philosophy** I wonder what there is about philosophy of animating. The Art and Science of Computer Animation by Stuart Mealing (1998) here. Daily Stanford article (2005) on Cartoons Simplify Chemistry with (largely) dismissive) comments by academics here How cartoons Work: The Cartoon Code by Randall P Harrison (1981) focussing on simplifying that relates to animating is here This is an area that needs further thinking. Most of the papers I have unearthed are on mechanics of animation production.	**Learner material:** **ChemSense** Nature of representation **Teacher material (other than that provided for learners):** **ChemSense** were initiators in tackling student produced animations using bespoke software Rob Toplis from UK carried out some work with pre-service teacher education students using ChemSense published by the RSC Maija Aksela and Jan Lundell from Finland have published work using Sparta

Modelling in chemistry – paper for the HIPST Project

John Oversby: University of Reading

Rationale for developing modelling capability

1. Most chemical explanations of macroscopic phenomena are based on submicroscopic models

A significant feature of the discipline of chemistry is that chemical explanations are based on entities existing at the nanometre level and below. Chemical explanation is also based fundamentally on electron rearrangements in ions, atoms and molecules, and these are not generally amenable to direct observation, even with instruments. Modelling of a wide variety is extensively employed in chemistry to make sense of the processes, which take place, and of the features of these entities, which affect the likelihood of chemical change.

2. Existing school chemical curricula teach chemical models as content to be learned

Science is based on "experimental evidence and models" to evaluate 'phenomena and events".

1. Pupils should be taught:

a) that atoms consist of nuclei and electrons
b) about a model of the way electrons are arranged in atoms
c) how the reactions of elements depend upon the arrangement of electrons in their atoms
j) how the rates of many reactions depend on the frequency or energy of collisions between particles

The quotes above are drawn from the consultation materials for the revised National Curriculum (Science) in England (DfEE, 1999), The revision, while maintaining in one section that learners should be taught that chemists use models, treats chemical models as static. They are also seen as equivalent to content in the chemical content section of the curriculum. The emphasis in the text on the phrase *'accepted models'* indicates this approach.

3. Existing school chemical curricula omit the process of modelling

... theories do not come automatically from evidence collected, but may involve creative thought or take the form of models

Implicit in this quote from the revised National Curriculum referred to above is that models simply exist, that they are there to be taught. Other sections from this document over-emphasise the need to teach the provisional nature of models, by focussing mainly on those which have changed, and neglecting to mention that most models are durable. While not changing the character of models as provisional, it is important to recognise that many chemical models have a long lifetime in an atmosphere of rigorous testing and use. Although it is hypothetically possible to imagine that a non-particulate model of chemical change could prove useful, in practice anyone who seriously criticised the general idea that chemical change involved particle entities would be gently led to one side and his or her sanity questioned. The quote also demonstrates an amazing view that models and creative thought are not related!

4. Existing assessment methods tend to ask for rehearsal of the taught use of models in explanations, or in slightly modified novel situations
In examination questions about bonding, especially ionic bonding, or about electrolysis, these are either aimed at testing whether students can use accepted models in a familiar context, or in a slightly modified context. The focus is on application of familiar knowledge or on rehearsal in the examination. I have not seen any question at secondary school level, which refers to the creation of the model itself. It may be felt that this is beyond the intellectual level of the learners at this stage but it seems not to be taught in higher education either. Clearly more careful work needs to be done to verify the generality of this claim but assessment of graduates on initial teacher education courses in England provides some corroborating evidence.

5. Chemical modelling, as a process, can promote commitment to and confidence in chemistry where other methods have failed
Oversby (1998a) has investigated this for pre-service primary student teachers and found this to be the case.

6. *Chemical modelling is an authentic* chemical *activity, and is intrinsically satisfying*
Oversby (1998) has made a case for the prime intellectual activity of chemical researchers being modelling. If this is accepted, then chemical modelling is authentic. The evidence for it being intrinsically satisfying is provided by the vast number of research articles based on chemical modelling which are published in the chemical literature. It is also intrinsically satisfying for some novices too (Oversby 1998b)

7. *Modelling is an intrinsic element in some National Curricula (eg England)*
A case for this is made above.

Chemical modelling capability

As with any new idea, some clarification of its meaning and extent is called for. The following is an attempt to put forward some of the major components and boundaries.

1. Recognition of models - representations of ideas, processes, events, systems, objects

Gilbert (1993) made a well-accepted delineation of the term model as a form of representation. The range of representation is broad and inclusive. The examples provided are not simply representative but include the major classes.

2. *Recognition of characteristics of good models* (based on Oversby, 1998b)

In this paper only a very brief indication of the issues is attempted.

a) Representational features - points of correspondence and non-correspondence. Models do not exactly correspond to the original, otherwise it would be the original. Explicit recognition of those aspects that correspond to the original is not always recognised. There will be many aspects that do not correspond but here is meant those aspects that might give rise to confusion or misunderstandings.

b) Analogical mapping - drawing on features expected to be in common between the model and the original.

c) Role in explanations - models are a common and essential component of chemical explanations

d) Human creation - models are the product of creativity, of synthesis and are often aesthetic.

e) Types of models - avoiding the tendency to think only of computer-based molecular modelling and ignoring non-traditional forms such as role-play and poetry. In chemistry, models include word equations, many drawn forms and prose descriptions.

f) Progression in modelling - based on both cognitive psychology thinking (eg progression from concrete to abstract) and natural thinking in chemistry about comparing qualitative and quantitative approaches.

g) Coherence with related models - idiosyncratic models tend to be shunned in chemistry.

h) Clear and systematic failure in explanations - for example, the ideal gas law fails not in a random way but in a manner which promotes modifications which possess rationality. The models created to modify the ideal gas law indicate significant features of the entities, such as their finite size and the existence of attractive forces.

i) Fruitfulness in exploring data from phenomena - the models for dissolution of ionic solutes have promoted the use of data such as measurement of energy changes, entropy changes, and dielectric constants in order to develop the hydration model further.

j) Predictive power in novel situations - the development of generalised kinetic models of organic substitution reactions has lead to greater confidence in predicting products from chemical reactions.

k) Simplicity - the simple ligand model for inorganic complexes has extended the range of data that can be explained using this model.

l) Quantitative if possible - - the transition state model of chemical kinetics has proved useful in explaining why the relation between absolute temperature and rate of chemical reaction is exponential. Such an approach leads to stronger tests of underlying models.

3. *Contexts for demonstrating modelling capability*

a) Use of existing models in familiar contexts
b) Use of existing models in novel contexts
c) Creation and use of new models in familiar contexts
d) Creation and use of new models in novel contexts

These are self-explanatory but as yet there is no understanding of whether learners find it easier to appreciate modelling if working within their personally created models, or if working with the accepted models of scientists.

Modelling for teachers Scholarship reading

1. Paper (from UK Lower Secondary Strategy) on using models in science teaching
2. Theodore Christofilis & Margarita Kousatana abstract paper on models in science education
3. Reality, Truth and The Logic of Science: Exploring Students' Views About Scientific Knowledge by Abhijeet Bardapurkar, Mumbai, India here
4. We, teachers of chemistry, have become teachers of the history of chemistry… but which type of history must we teach? by José A. Chamizo
5. NZ teaching with models
6. Research on models in teaching chemistry (RSC)
7. JCE Chemical affinity diagram of 18th century (a kind of chemical equation)
8. David Knight includes a little on chemical equations in his Hyle article
9. The role of submicroscopic and symbolic representations in chemical explanations Treagust, Chittleborough & Mamiala
10. PALAVA project: submicroscopic representations for gases in syringes by Oversby
11. Gail Chittleborough's thesis Chapter 1
12. Mental models web site
13. Wikipedia mental models
14. Promoting understanding of chemical representations: Students' use of a visualization tool in the classroom Authors: Wu, Hsin-Kai; Krajcik, Joseph S.; Soloway, Elliot
15. Philosophy for Children site.
16. Jean Beguin - first chemical equation 1615

Overview of the Paper Tools (Modelling) Topic for Teachers

The theme of modelling is pervasive through the whole of science education. I have chosen to restrict the topic to chemical equations, largely because I have a lot of material on it both historical and philosophical, and it is central theme in school chemistry in all countries, but also because it exemplifies ideas about representation that are common across all the sciences. It also bridges the tension between conceptual understanding and quantitative calculations that are present in chemical education and chemistry.

Modelling through chemical equations

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Introduction to modelling at macroscopic and sub-microscopic levels: pressure in syringes (see PALAVA experiment below) THE PALAVA PROJECT – A METHOD OF ASSESSINGMODELLING CAPABILITY The survey work is well described in this article.	**History:** Article on The Era of Alchemy by Greg Goebel, in the public domain; do read the section on The Rise of Scientific Ideas for comments about the challenges of studying gases when they can not be contained. The article suggests that 'the long-lost atomic ideas of Democritus, who had correctly envisioned air as particles bouncing around in a vacuum' 'had resurfaced in the 15th century, and made a convert in the form of the French philosopher Pierre Gassendi (1592:1655), who spread the word'. A biography of Democritus is in Wikipedia Another biography of Democritus (Stanford Encyclopedia of Philosophy). Whether Democritus understood a vacuum (void) in the same way that we do now is debatable. Both Boyle and Toricelli in the 17th century created models of air based on quantitative data about air, e.g. the effect of pressure on air volume at a fixed temperature. Bernoulli developed these in 1738. **Philosophy** Democritus' views on epistemology, and whether senses can discover truth are discussed in the Wikipedia biography . This is further discussed in the Stanford text. The Stanford text contains an excellent discussion of ancient Greek philosophy in a reasonably accessible tone, for teachers. The ideas of the Greeks came from thinking, i.e. philosophy, not empirical and practical investigation. A Wikipedia biography of Pierre Gassendi is available but is tough reading, in line with the ideas	**Avoidance of whiggishness:** Looking at whether Democritus' ideas about a void and atoms are the same as today.

	of the time!	
Clues about compounds: law of constant composition as an indicator of atoms Clues about law of conservation of mass: efforts to represent atoms.Third level of representation ie symbolic. Issues about balancing equations.	**History**: Law of constant composition (definite proportions) from Wikipedia See pictures of balances from Science and Society picture library. Note Ramsden's balance from late 18th century, and the 'self-indicating balances designed by Da Vinci, 1452-1519'. Lavoisier computed masses, using an accountant's expertise (he did work as in the *Ferme Generale* collecting taxes for the French government, for which he was beheaded in 1794 on the guillotine) and his tables (reproduced here) look very similar to financial tables. 'The oldest surviving balance used for a published series of chemical experiments is said to be that used by ... Joseph Black', described in his doctoral thesis of 1754 (quoted here). Black's balance had a sensitivity of about 1 in 14000) Jon Berzelius' fundamental work is written in Wikipedia, including his symbolic forms that represent elements and atoms. Chemical Heritage Foundation on Lavoisier **Philosophy**: Induction is the process by which ideas about atoms were proposed to explain constant composition of compounds. Explanation from Intute web site Given incompleteness of chemical reactions, can equations be balanced? A major problem in traditional quantitative analytical chemistry was to ensure firstly that the materials used were pure, and secondly, that the reaction used for calculations proceeded 100% as written.	**Avoidance of whiggishness:** From Wikipedia - ' The law of definite proportions might seem obvious to the modern chemist, inherent in the very definition of a chemical compound. At the end of the 18th century, however, when the concept of a chemical compound had not yet been fully developed, the law was novel. In fact, when first proposed, it was a controversial statement and was opposed by other chemists, most notably Proust's fellow Frenchman Claude Louis Berthollet, who argued that the elements could combine in any proportion.[3[[http://en.wikipedia.org/wiki/Law_of_definite_proportions#cite_note-2|]]] The very existence of this debate underscores that at the time, the distinction between pure chemical compounds and mixtures had not yet been fully developed.[4[[http://en.wikipedia.org/wiki/Law_of_definite_proportions#cite_note-3|]]] This part of chemistry marked progress in manufacture of chemical balances) (Lavoisier had his balances made in the Netherlands by (biography Nicolas Fortin)and Pierre Bernard Megnie) **Learner material:** Law of constant composition Nature of philosophical induction Chemical Heritage practical on fermentation. It is aimed at early undergraduate level. Chemical Heritage practical on

		magnesium burning. A Chemical Heritage paper on Lavoisier's instruments as Objet's D'Art. **Teacher material (other than that provided for learners):** Non-stoichiometric compounds from Wikipedia
Chemical change and its representation in equations. Chemical equations v mathematical equations	**History** First chemical equation (1615) by Beguin Biography of Cullen (1710-1790) (used diagrams as chemical equations) Biography of Lemery (1645-1715). **Philosophy** Nature of representation Stanford - Mental Representation Nature of scientific modelling What is the nature of the distinction between chemical and physical change? Is it helpful, powerful or simply plain wrong? Some of the history of its introduction may be a good start.	**Avoidance of whiggishness:** Development of systems of chemical representation took place over a long period of time. The challenge was to infer sub-microscopic explanations from macroscopic phenomena. **Learner material:** Beguin and Cullen's early attempts to write chemical equations. John Dalton's symbols (see Wikipedia) **Teacher material (other than that provided for learners):** Mental modelling
Signs in chemical equations; origin and use	**History** History of + sign in chemical equations History of chemical arrows Braille chemical signs and symbols **Philosophy** Semiotics for beginners - nature of signs	**Avoidance of whiggishness:** The impact of external influences such as printing technology on conventions for printing chemical equations demonstrates the complex interchange between the rationality of chemists making decisions about their discipline and others. **Learner material:** History of signs in chemical equations, focusing on + and = signs, as opposed to arrows, based on Oversby papers. **Teacher material (other than that provided for learners):** Semiotics for beginners - nature of signs All of the web sites visited on 2 Dec 08, by Googling Chemical Notation, focused only on expressions of formuae,

		and not on the signs, such as arrows, and +. The Braille site is mainly concerned with arrows. there are many computer sites concerned with mark up of chemical formulae but not signs.
Computer animations of chemical processes - a step in representation	**History** First of an article on the history of animating. Wikipedia full article on history of animation **Philosophy** I wonder what there is about philosophy of animating. The Art and Science of Computer Animation by Stuart Mealing (1998) here. Daily Stanford article (2005) on Cartoons Simplify Chemistry with (largely) dismissive) comments by academics How cartoons Work: The Cartoon Code by Randall P Harrison (1981) focussing on simplifying that relates to animating This is an area that needs further development. Most of the papers I have unearthed are on mechanics of animation production.	**Avoidance of whiggishness:** This topic is modern and whiggishness is not a problem. **Learner material:** **ChemSense** Nature of representation **Teacher material (other than that provided for learners):** **ChemSense** were initiators in tackling student produced animations using bespoke software Rob Toplis from UK carried out some work with pre-service teacher education students using ChemSense published by the RSC Maija Aksela and Jan Lundell from Finland have published work using Spartan in CERP

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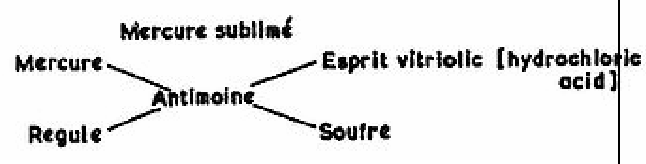
Paper Tools



Beguin's 1615 reaction diagram, the first-ever chemical equation: reaction of corrosive sublimate ($HgCl_2$) with sulphide of antimony (Sb_2S_3)
There are lots of different kinds of chemical equations!

A precision balance scale for weighing silver and gold located on display at the Historic Archive and Museum of Mining in Pachuca, Mexico. Balancing were often used in medieval times for finding the purity of precious metals such as gold and silver (assaying)

Weighing

History From Wikipedia and other sources

Simple balances were used as early as 5000 B.C. So long is their history that the very word "balance" comes from the Latin word *bilanx* which means "two pans." The modern analytical balance originated during the mid-18th century, when the Scottish chemist Joseph Black developed the technique of using a lightweight, rigid beam supported on a knife-edged fulcrum. The accuracy achieved by this innovation far surpassed that of any other weighing device.
(from NIH Stetten Museum http://history.nih.gov/exhibits/balances/index.html)

Lavoisier's most sensitive Fortin balance was accurate to 1 part in 400,000. Unlike in physics, much less information is available on early chemical instruments, perhaps because they had less prestige. Glass equipment was only used once, although Lavoisier’s glass equipment had brass connectors that could easily be assembled and dismantled.

Below is part of a letter written by the chemist Dr Black to James Smithson Esq. ‘describing a very sensible balance’ September 18th, 1790 at http://www.nls.uk/scientists/pageturner.cfm?id=74630410
‘The apparatus I use for weighing small globules of metals, or the like, is as follows: A thin piece of fir wood not thicker than a shilling, and a foot long, 3/10 of an inch broad in the middle, and 1½/10 at each end, is divided by transverse lines into 20 parts; that is, 10 parts on each side of the middle. These are the principal divisions, and each of them is subdivided into halves and quarters. Across the middle is fixed one of the smallest needles I could procure to serve as an axis, and it is fixed in its place by means of a little sealing wax.’

Features of a good balance

Sensivity: either being able to measure the smallest mass, or being able to respond to the smallest mass difference

Precision: being able to respond to the smallest mass difference.

Accuracy: being able to measure the true mass

Reliability: being able to give the same mass measurement time and again

Design of a good balance

Sensitivity: reduce friction by having a sharp and hard wearing balance point, having long arms

Precision: reduce friction by having a sharp and hard wearing balance point, having long arms

Accuracy: use good reference weights, correct for buoyancy, avoid air gusts, which push the pan up or down, avoid dust settling on the pan or object, reduce friction that prevents balance settling down, calibrate correctly, avoid temperature changes that can cause misalignment by thermal expansion or contraction, avoid magnetic fields, avoid electrostatic fields such as those from feet scuffing on carpets or plastic floors, avoid chemical reaction between air and the balance (corrosion) or the articles being weighed, avoid condensation onto or evaporation of moisture from weighed articles, avoid air convection currents e.g. by working in a vacuum, avoid places where gravitation might be affected, avoid external vibration e.g. from assign trucks and trains

Reliability: reduce friction that prevents balance settling down.

Historical development and importance of conservation of mass (Wikipedia)

Beginnings of the theory of conservation of mass were stated by Epicurus (341–270 BC). Describing the nature of the universe, he wrote: "the sum total of things was always such as it is now, and such it will ever remain," and that nothing is created from nothing, and nothing that disappears ceases to exist. An early yet incomplete theory of the conservation of mass was stated by Nasīr al-Dīn al-Tūsī (1201–1274) during the 13th century. He wrote that a body of matter is able to change, but is not able to disappear.
The principle of conservation of mass was first outlined clearly by Antoine Lavoisier (1743–1794) in 1789, who is often for this reason referred to as an initiator of modern chemistry. However, Mikhail Lomonosov (1711–1765) had previously expressed similar ideas during 1748 and proved them by experiments. Others who anticipated the work of Lavoisier include Joseph Black (1728–1799), Henry Cavendish (1731–1810), and Jean Rey (1583–1645).[3]
Historically, the conservation of mass and weight was obscure for millennia because of the buoyant effect of the Earth's atmosphere on the weight of gases. For example, since a piece of wood weighs less after burning, this seemed to suggest that some of its mass disappears, or is transformed or lost. These effects were not understood until careful experiments in which chemical reactions such as rusting were performed in sealed glass ampoules, whereby it was found that the chemical reaction did not change the weight of the sealed container. The vacuum pump also helped to allow the effective weighing of gases using scales.

There is a YouTube video
http://www.youtube.com/watch?v=J5hM1DxaPLw&NR=1

Landolt's original paper
Landolt, H. *Z. physik. Chem.*, **1908**, *64*, 581
Landolt's experiments have been studied more recently:
www.scientificexploration.org/journal/jse_08_2_volkamer.pdf

This is also tied up with the invention and refinement of analytical balances.
http://history.nih.gov/exhibits/balances/

Play script for Antoine and Marie-Antoinette Lavoisier on the Law of Conservation of Weight (Mass) over dinner one night in 1788, 6 years before Antoine was beheaded at the guillotine.

AL: Dear Marie-Antoinette, I have been thinking about the ideas that are going round about weight changes during chemical changes. You know that other respected chemists have been thinking about these too.
M-AL: Which chemists are these my dear?
AL: Well, firstly there is Mikhail Lomonosov, the Russian Professor of Chemistry at the Russian Academy of Science. He said: "Today I made an experiment in hermetic [sealed] glass vessels in order to determine whether the mass of metals increases from the action of pure heat. The experiments– of which I append the record in 13 pages– demonstrated that the famous Robert Boyle was deluded, for without access of air from outside the mass of the burnt metal remains the same." He has written to Leonhard Euler to say that: "All changes in nature are such that inasmuch is taken from one object insomuch is added to another. So, if the amount of matter decreases in one place, it increases elsewhere." Lomonosov wrote so in his dissertation of 1760.
M-AL: But this is only one person. Are there really any more?
AL: Ah, but Joseph Black, the Scottish Professor of Medicine has also been weighing the starting materials and the finished materials in his experiments, but I must say that his balance was not as sensitive as mine. I have also heard that Henry Cavendish, born of British aristocracy, has studied changes in weight using air, but he is so shy that nothing has yet been published by him. Jean Rey, the French physician and chemist, studied heated lead and tin, and found they weighed more afterwards. He said this was because the extra weight had come from part of the air.
M-AL: So Antoine, you are the only one who has been thinking clearly that when a chemical change takes place, if you could collect and weigh everything before and afterwards, the totals would be the same.
AL: That is so, but in some of my experiments, the weights are not exactly the same, although they are very close together. I think it is some problem in making correct measurements, or losing something from my glassware, that causes these small differences. I will search and see if I can find the small mistakes I have made. I am sure the weight must always stay the same, even if my results are not always supporting this.

M-AL: Well, my dear, you must publish this idea, and I will do the drawings of your equipment. Should I draw your super balance you bought from Monsiour Fortin, in Holland?
AL: No my dear. Balances are very common, and everyone knows what they look like! Let us do the writing and drawings tomorrow.

Law of definite proportions (Law of constant composition)
From Wikipedia, the free encyclopaedia

In chemistry, the **law of definite proportions and also the elements** states that a chemical compound always contains exactly the same proportion of elements by mass. An equivalent statement is the **law of constant composition**, which states that all samples of a given chemical compound have the same elemental composition. For example, oxygen makes up $^8/_9$ of the mass of any sample of pure water, while hydrogen makes up the remaining $^1/_9$ of the mass.

History

This observation was first made by the French chemist Joseph Proust based on several experiments conducted between 1798 and 1804. Based on such observations, Proust made statements like this one, in 1806:

> "I shall conclude by deducing from these experiments the principle I have established at the commencement of this memoir, viz. that iron like many other metals is subject to the law of nature which presides at every true combination, that is to say, that it unites with two constant proportions of oxygen. In this respect it does not differ from tin, mercury, and lead, and, in a word, almost every known combustible."
> Translated into Modern and Easy English:
> "I finish by deducing from these experiments a new natural principle or law of nature. This is that when iron combines with oxygen, two different compounds can be made. In each one, the proportion of oxygen is always the same. The same is true for tin, mercury and lead. This is the law of Constant Composition.

We should note that this Law is not only a natural principle, but separates compounds from mixtures. Mixtures have variable composition and compounds have a fixed composition. The law of definite proportions might seem obvious to the modern chemist, inherent in the very definition of a chemical compound. At the end of the 18th century, however, when the concept of a chemical compound had not yet been fully developed, the law was novel. In fact, when first proposed, it was a controversial statement and was opposed by other chemists, most notably Proust's fellow Frenchman Claude Louis Berthollet, who argued that the elements could combine in any proportion. The very existence of this debate underscores that at the time, the distinction between pure chemical compounds and mixtures had not yet been fully developed.

The law of definite proportions contributed to, and was placed on a firm theoretical basis by, the atomic theory that John Dalton promoted beginning in 1803, which explained matter as consisting of discrete atoms, that there was one type of atom for each element, and that the compounds were made of combinations of different types of atoms in fixed proportions.

Can you write a play script between Proust and Berthollet on this Law? We will publish some of them in this newspaper.

Representing formulae

This Wikipedia site has a detailed explanation of the history of the atomic theory, from Indian and Greek ideas to those of the 18th century. http://en.wikipedia.org/wiki/Atomic_theory. In this piece, we will start at the 18th century. A play script that places various historical characters at the same time shows how the ideas link.

Lavoisier produced his idea of Conservation of Mass in 1789. Proust provided us with the Law of Definite Proportions in 1799. Dalton gave us his ideas of Atomic Theory in 1803. Avogadro introduced the idea of molecules in 1811. Berzelius chose to represent elements by letters around 1808.

ThisWikipedia article tells about the history of molecules: http://en.wikipedia.org/wiki/History_of_the_molecule You will see that the story is complicated but that the ideas came at about the same time in history.

Play Script about Atomic Theory

AL = Antoine Lavoisier JLP = Joseph Louis Proust

JD = John Dalton AA = Amadeo Avogadro

JJB = Jöns Jacob Berzelius

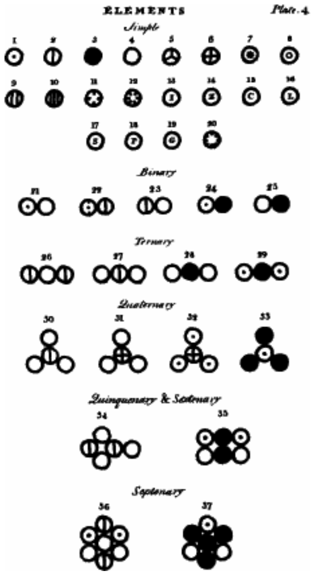
AL: I had been thinking that matter was made up of small particles called atoms. When I discovered that the total weight of things did not changed significantly in a closed flask, however much they changed in other ways, I felt that my theory of atoms explained this very well. It was just as well that I had my new sensitive balance from Fortin to work with. It was just that the atoms simply rearranged but stayed the same in number. So, I felt that the idea that weight remained constant, and I started to search for errors in my data where this did not fit.

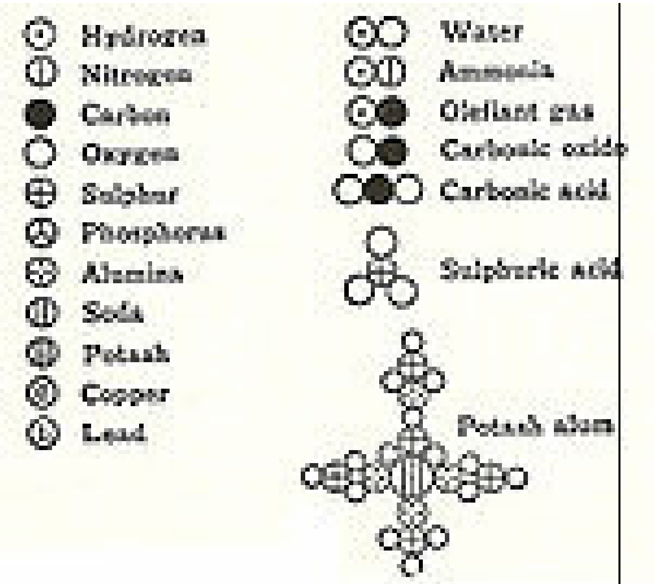
JLP: Thank you Antoine for that start to our thinking about atoms. I explained the Law of Definite Proportions when thinking that the weight of all atoms of the same element must be the same. If this then was the case, and I then assumed that the atoms always connected in the same pairs, trios, etc, then the composition by weight would always be the same. Let us imagine the black oxide of copper. Then it will always be made up of one atom of copper and one atom of oxygen. So, it will always have the same composition. Unfortunately, the information we have about the relative weights of each atom is so bad these days. We will have to wait until some chemist is able to analyse these materials better, and find the combining weights.

JD: I have managed to analyse more materials and compare my data with that of other chemists. The experimental challenges were great, though. No doubt, someone else will come along with more accurate weighing. I found that the hydrogen atom is the lightest one. For this reason, I have decided to make the weight of one atom of hydrogen to weigh one unit. Here is my list:

Element (modern name)	**Relative weight**	**21st century**
Hydrogen	1	1
Azote (nitrogen)	5	14
Carbone or charcoal	5	12
Oxygen	7	16
Phosphorus	9	31
Sulphur	13	32
Magnesia (magnesium)	20	24
Lime (calcium)	23	40
Soda (sodium)	28	23
Potash (potassium)	42	39
Strontites (strontium)	46	
Barytes (barium)	68	
Iron	38	
Zinc	56	
Copper	56	
Lead	95	
Silver	100	
Platinal (platinum)	100	
Gold	140	
Mercury	167	

I have also prepared some symbols to represent compounds. You will see that some are simple, and some have two atoms joined together (binary), some three (ternary), some four (quaternary), some five (quinquenary), some six (sextenary) and some seven (septenary). I have found these from the atomic weights of the compounds that I have determined.





JJB: John, I read your paper although it took a long time to reach me in Sweden because of the war that was going on. Our printers have found some problems with your symbols. You see, they have the type in hard metal, in boxes called cases. They put the small letters in the lower cases and the capital letters in the upper cases. They place these metal letters in frames, spread ink on them, and then press the paper onto the inked frames. Unfortunately, they have to make your symbols specially and this increases the costs of printing too much. I have chosen to use the normal capital letters for the element symbols. Where more than one element starts with the same letter, such as carbon and calcium, I use a second small letter for one of them. So carbon is represented by C, and calcium by Ca. I have used the Latin names for those elements known in history. For a compound such as carbonic acid gas, I chose to use CO^2 but Gmelin who publishes my work in his journal prefers to use CO_2. I often use the + sign to mean combined with, as chemists of these days do. It is sometimes easiest to imagine that there is just one of each atom in each particle of compound, so this would be Cu+O, of copper the oxide.

AA: What an excellent idea Jöns for representing atoms using the letters of the element names! I am sure it will catch on. I have discovered a little problem with John Dalton's atomic weights. Some elements are not made of simple atoms, such as H, O and N. They have compound atoms such as H_2, O_2 and N_2. This is why some of John's weights are just half of what they should be. I will call these new compound atoms 'molecules', from the Latin for little heap.

Interpreting formulae

Formulae are not just random letters, or made from rules that anyone can simply learn. Formulae have rich meanings as this section will make clear.

Subscripts and superscripts

19th century chemistry textbooks were not consistent in their use of subscripts (e.g. H_2) or superscripts (e.g. H^2) but they all had them after the symbol. It seems that this was done to make chemistry different from mathematics, not just to make chemistry learning difficult! So, in mathematics, two lots of a are 2a but in chemistry two lots of hydrogen was H_2 or H^2 depending on who the author was. Some chemist had a different symbol for doubling, a symbol with a line through it (e.g. Ħ was similar to H_2) but this only lasted for a while. In the early 1800s, reading formulae was also challenging! By the early 1900s, only the French were using superscripts in textbooks and journals. Today, all chemists use subscripts.

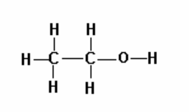
Symbols of elements

Berzelius invented the system of using a capital letter e.g. H, or a capital followed by a small letter e.g. Ca. Some symbols were based on the Latin name, e.g. Cu for copper (Latin Cuprum) or Pb for lead (Latin Plumbum). Some symbols were based on continental names e.g. Na for sodium or natrium, or K for potassium or kalium. This was an accepted convention.

The particles that make up chemicals can not be seen with microscopes. We call them sub-microscopic particles. The sub-microscopic particle of many elements is just a single atom. For some elements, the sub-microscopic particle has two or more atoms joined together e.g. H_2, O_2, N_2, Cl_2, P_4, S_8. There is not an obvious pattern to which ones have multiple atoms.

Representing compounds

There are so many different kinds of formulae! Each of them has a different set of purposes. As an example, I will consider different formulae for ethanol. Antoine Lavoisier worked out the composition for ethanol by burning a weighed quantity and weighing the carbon dioxide and water made from it. This was a tricky task but he was helped by having a good balance. From the weight composition chemists can work out the empirical formula. The table below gives some interpretation of what each formula might show. These are only some of the features. The eagle-eyed might detect other features special to each kind of formula.

	Empirical	**Condensed**	**Displayed**
It looks like	C_2H_6O	CH_3CH_2OH	
What does this formula show?	The simplest number of each atom in one molecule: two of carbon, six of hydrogen, and one of oxygen	As the empirical formula plus: a) the two carbons are joined; b) the oxygen is joined to one of the carbons; c) the hydrogen atoms are split up between the two carbon atoms and the oxygen; d) there are two kinds of hydrogen, those joined to carbon and the one joined to oxygen.	As the condensed formula plus: a) the lines represent a kind of bond; b) the bonds are all single bonds; c) each hydrogen is joined to only one other atom; d) each carbon is joined to four other atoms; e) the oxygen is joined to two other atoms.