Models and Molecules: Representation in the Work of John Dalton

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Abstract This paper briefly addresses representation in early nineteenth-century chemistry with reference to the work of John Dalton (1766-1844). The focus will be on the design and implementation of Dalton's atomic symbols and threedimensional molecular models. It will first examine the individual symbols presented in *A New System of Chemical Philosophy* before attempting to categorize them according to design. The discussion will then shift to the ways in which he manipulated the symbols alongside the posters and handbills he employed as pedagogic tools. Dalton's wooden balls were useful musing and pedagogic aids that helped him to visualize his two-dimensional construction. In the final section, their design and function will be discussed; particular attention will be given to their spatial arrangements to suggest he was one of the earliest stereochemists. Finally, conclusions will be drawn on his deductive reasoning to show that his visual thinking was apparent in his symbols and models.

Resumo O presente artigo aborda o tema da representação na química dos inícios do século XIX, por referência à obra de John Dalton (1766-1844). A nossa atenção incidirá no *design* e na implementação dos símbolos atómicos e dos modelos moleculares tridimensionais. Primeiro são examinados os símbolos individuais apresentados em *A New System of Chemical Philosophy* antes de os categorizarmos de acordo com o *design*. Seguidamente, discutir-se-ão os modos através dos quais Dalton manipulou os símbolos, bem como os posters e folhetos que utilizou como instrumentos pedagógicos. As bolas de madeira de Dalton foram instrumentos pedagógicos úteis que o ajudaram a visualizar a sua construção bidimensional. Na secção final, será discutido o seu *design* e função; é dada especial atenção à sua distribuição espacial, sugerindo-se assim que foi um dos primeiros estereoquímicos. Finalmente, serão extraídas conclusões quanto ao seu raciocínio dedutivo para mostrar que o seu pensamento visual aparecia já nos seus símbolos e modelos.

Introduction

In this paper I will briefly discuss representation in early nineteenth-century chemistry with reference to the work of John Dalton (1766-1844). The focus will be on the design and implementation of Dalton's atomic symbols and three-dimensional molecular models. I will first examine the individual symbols presented in *A New System of Chemical Philosophy* (1808-1827) and attempt to categorize them according to design.

The discussion will then shift to the two-dimensional representations of compounds Dalton drew using his individual symbols. I will examine the ways in which he manipulated the symbols and in doing this, the posters and handbills he employed as pedagogic tools will be presented.

Dalton's wooden balls were useful musing and pedagogic aids that helped him to visualize his two-dimensional construction. In the final section, their design and function will be discussed. I will pay particular attention to their spatial arrangements to suggest he was one of the earliest stereochemists. Finally, I will draw conclusions on his deductive reasoning and hope to show that his visual thinking was apparent in his symbols and models.

What is a symbol?

For the purpose of this study, it is useful to explain what I mean when I refer to the term 'symbol'. I associate the term with the images and pictograms Dalton (and others) created to represent the chemical elements and subsequent compounds. Defining the term 'symbol' can be problematic. On a basic level, a symbol is a sign or a graphic mark that represents something. In this paper, it refers to a printed or hand-

Rachel Dunn

drawn image representing a chemical substance, so it has a specified meaning. If the image does not represent anything it is merely a meaningless sign.¹ The social anthropologist Sir Edmund Leach wrote that, "a sign or a symbol only acquires meaning when it is discriminated from some other contrary sign or symbol."² In this respect, Dalton's symbols only take on a meaning (that is useful to the scientist) when seen as part of a complete system. Taking Leach's idea, I would suggest that the tables and compound symbols Dalton produced enabled the individual images to be compared and thus acquire meaning. Leach believed that symbolic representation is a relation between three elements: the concept in the mind, sense image and an object in the external world. He pointed out that an object (in our discussion, a chemical substance) in the external world is connected with a sense image (e.g. a visual symbol) by cultural convention, and this relationship is always arbitrary and metaphoric.³

The historian Maurice Crosland wrote that early chemical symbols were originally derived from pictograms, abbreviations and arbitrary signs.⁴ The derivation of symbols changed towards the eighteenth century when chemists preferred to analyze symbols in search of a rational justification for each stroke.⁵ Symbols often represented the name of a substance rather than the substance itself. This then followed that symbols often had a literal meaning and, when combined, represented a substance with a compound name.⁶

The meaning of a sign can change over time, with the situation, and be manipulated by the author or user, so consistency is an important factor. Dalton dallied with his symbols over the five-year

¹ Korzybski, 2000, 79.

² Leach, 1976, 49 quoted in Burke, 2005, 5.

³ Leach, 1976, 19 quoted in Mach, 1993, 26-27.

⁴ Crosland, 1962, 232.

⁵ Crosland, 1962, 233.

⁶ Crosland, 1962, 235.

period from their first recording in his notebook in September 1803 (see Figure 1), most notably addressing the representations of hydrogen, oxygen, sulphur and gold. Once he published the first volume of *A New System of Chemical Philosophy* in 1808, the symbols were fixed and their form remained unchanged through subsequent editions.

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Figure 1: Initial iteration of Dalton's symbols (from his notebook, September 1803, facsimile reproduction from Roscoe and Harden, 1896, 29).

Dalton's symbols

Dalton's atomic symbols represent one atom of each element; he subsequently used the term 'compound atom' to refer to ultimate particles of compounds. Originally drawn by hand, the symbols are pictorial as they are visual tools used to represent given substances in Dalton's notebooks, lecture notes and correspondence (see reproductions in Roscoe and Harden (1896) and archives of The Royal

Rachel Dunn

Society and John Rylands University Library, Manchester). They were later standardized and reproduced in Dalton's books and lectures. Dalton's symbols sometimes suggested pictorially a property or a resemblance.⁷ For example, the symbol for Sulphur is similar to the symbol for Sulfur (sic) in alchemical tables with the use of a cross. As Dalton believed that atoms were surrounded by an outer atmosphere of heat, he surmised that every atom would be more or less spherical in shape.⁸ The atoms were represented in circles, as a circle is the twodimensional representation of the sphere.



Figure 3: Dalton's symbols from *A New System of Chemical Philosophy* (1808), plate 5, no page number.

⁷ Crosland, 1962, 28.

⁸ Rouvray, 1995, 54.



Figure 1: Dalton's symbols from A New System of Chemical Philosophy (1808), plate 6, no page number.

Once he had decided on a circular form, he had to compile distinguishing marks to differentiate the individual atoms. For this Dalton used a mixture of letters and patterns enclosed within the circles (see Figures 2 and 3). The letters he used were the initial letters of the English names of the elements. It was surprising that Dalton used symbolic notation incorporating letters given his "great repugnance" to Berzelius' alphabetical symbols.⁹

Aside from those designated by initial letters, where did the designs come from? Dalton invented some of the symbols whilst others show signs of earlier influences. For example, the symbol for copper was the same as Hassenfratz and Adet whereas the full circle

⁹ Roscoe and Harden, 1896, 45.

Rachel Dunn

for carbon was original. In a similar way to Geoffroy, some of Dalton's symbols had their origins in alchemy. Dalton borrowed the use of pictures instead of letters from alchemy, but with one important distinction, he meant each individual picture to represent particular quantities of atoms.¹⁰

Looking at similarities and groupings, in discussion with Dalton's symbols, I would classify them in three categories: (1) abbreviations (e.g. G for Gold), (2) symbolic signs (reminiscent of the substance's properties or form, e.g. a coloured black circle for Carbon) and (3) original signs (e.g. the symbol for Glucine). Dalton's symbols appeared to fall into these three categories, with more original or arbitrary signs present in his earlier symbols and more abbreviations in later lists.

As Dalton's symbols were a scientific tool, they represented the iterative nature of scientific investigation as they changed over time as the system developed from notebook to publication. For example, Hydrogen and Oxygen originally had the opposite symbols. The symbol for Sulphur was similar to the symbol for Sulfur (*sic*) in alchemical tables with the use of a cross. If we examine Dalton's symbols for Hydrogen, Oxygen and Carbon, it is possible that he chose the simplest symbols, (a circle with a central dot, an empty circle and a solid circle) for these most commonly used elements. This would aid their use in handwritten texts and make dies or engraving blocks easier and possibly cheaper to produce. Such simple symbols also suggest a leaning towards the Quaker notion of simplicity, to which Dalton subscribed, or could simply recognise the need for brevity in recording scientific data. Despite the fact pictorial symbols represented a typographical problem, Dalton persisted with them.

¹⁰ A more in-depth discussion of the development of Dalton's symbols is given in Maurice Crosland's 1962 study, *Historical Studies in the Language of Chemistry*. New York, Dover, 256-264.

Manipulating the symbols: making compounds

Alongside his symbols for the atomic elements, Dalton drew twodimensional representations of compounds using his individual symbols. He placed symbols next to each other in an order believed to be the actual spatial arrangement of the atoms in the compound. In creating these compounds he assumed the simplest possible formulas, e.g. water as a binary compound, HO, rather than, as we now know, H₂O. Essentially, Dalton had to make assumptions as to the numbers of atoms that combined to form each compound. This deductive reasoning has been praised by observers such as Roscoe and Harden, but criticised by others, such as David Knight, who recognised that Dalton's two-dimensional constructions failed to connect with the work of contemporaries such as William Hyde Wollaston who was engaged in work on the composition of crystals.

The creation of a set of symbols to represent each element almost acts as an alphabet, but to make effective use of it, Dalton needed to write words using it, through the creation of compound symbols. Dalton's symbols for compounds were made up of easily recognizable, unaltered symbols that could be deconstructed to their constituent parts. In this respect, I put forward that Dalton's compounds were useful as the reader could recognize the elements involved and draw schematic interactions.

Dalton himself employed his symbols in this capacity. However, their very structure made them cumbersome and led to difficulty in writing formulae for complicated compound atoms, meaning they were impractical and often imposed a spurious structure on some compounds, e.g. alum.¹¹ It did mean that the reader could visually interpret the chemical formula, e.g. alum is constructed of one atom

¹¹ Rouvray, 1977, 28.

of potash, four of alumine, five of sulphur and fifteen of oxygen (see Figure 3 from *A New System of Chemical Philosophy*). Composing a new symbol for each compound would have been easier, but Dalton maintained his construction of compound atoms for years to come, as seen in his diary and lecture notes.¹² Using this symbolic representation of invisible atoms, they could be combined on paper, discussed and corrected. This paper modelling enabled atoms to be manipulated, creating interactions that could then be confirmed or denied by experiment; this theoretical chemistry could be considered ahead of its time.

Employing the symbols in teaching materials

Dalton's symbolic notation described above enabled him to easily communicate his ideas. Fellow chemist Thomas Thomson publicized Dalton's symbols in his 1807 work, *System of Chemistry*, the year before Dalton first published them in *A New System of Chemical Philosophy*.¹³ He later wrote that representing atoms by Daltonian symbols aided clarity.¹⁴ Thomson subsequently arranged for Dalton to lecture in his classroom in Edinburgh in April 1807 during a tour of Edinburgh and Glasgow. In his Scottish lectures, Dalton used various posters, including one that presented symbols and relative weights of the first twenty substances included in the first volume of *A New System*. The posters were quite large, being 19" by 26 ½". Gee, Coward and Harden described fifty-three lecture diagrams that refer to the atomic theory (for an example, see Figure 4).¹⁵

¹² As discussed by Roscoe and Harden.

¹³ Thomson, 1807, 429-540.

¹⁴ Thomson, 1830, 291.

¹⁵ Gee et al. 1915.



Figure 4: Photograph of Dalton's lecture poster "*Elements*" for his Scottish lectures in 1807 (from Coward, 1927, 29).

The posters were considered lost until just before the First World War when some were discovered in a cupboard at the Manchester Literary and Philosophical Society. There were about one hundred and fifty altogether, which Dalton used in teaching, all apparently prepared by his own hands. Some of them illustrated Dalton's ideas of the chemical constitution of substances, and his exposition of the atomic theory. There can be little doubt that the posters were prepared in 1806 or 1807 for illustrating the lectures delivered in Scotland in April of the latter year.¹⁶ It is with regret that the documents were lost, along with a considerable amount of the Dalton archive, following a fire during the Second World War.

Dalton allegedly made greater use of his symbols in oral presentations than in his published works and laboratory notebooks.¹⁷

¹⁶ Coward, 1927, 29.

¹⁷ Gee et al., 1915, 41.

Rachel Dunn

This is quite remarkable as he frequently employed his symbols in written work.¹⁸ In an essay read to the Manchester Literary and Philosophical Society in October 1830, Dalton discussed the necessity for the lecture posters in explaining the symbols of atoms and their arrangement in compound atoms:

All this would have been very difficult to convey to a large and promiscuous audience without suitable diagrams.¹⁹

He also issued handbills at, among other lectures, a BAAS meeting and an 1835 lecture in Manchester.²⁰ An example of the handbill given at the 1835 meeting is shown in Figure 5.



Figure 5: Copy of the handbill issued at the Manchester Mechanics Institution in 1835 (from author's personal collection).

¹⁸ Gass, 2007, 371.

¹⁹ Dalton, paper read to the Man Lit & Phil 15 October 1830. Fire damaged manuscript reproduced in Thackray, 1972, 96.

²⁰ Thackray, 1972, 119; Smyth, 1998, 59.

One of the most important aspects of Dalton's science was that he thought in three-dimensions with respect to atomic dynamics. In 1810, he engaged his friend Peter Ewart (an engineer who worked for Bolton and Watt) to produce some three-dimensional wooden models to assist in his teaching. He described their construction, thus:

My friend Mr Ewart, at my suggestion, made me a number of equal balls, about an inch in diameter, about 30 years ago; they have been in use ever since, I occasionally showing them to my pupils. One ball had 12 holes in it, equidistant; and 12 pins were stuck in the other balls, so as to arrange the 12 around the one and be in contact with it: they (the 12) were about 1/20 inch asunder. Another ball, with 8 equidistant holes in it, and they (the 8) were about 3/10 of an inch asunder, a regular series of equidistant atoms. The 7 are an awkward number to arrange around 1 atom. The six are an equidistant number of atoms, 90 degrees asunder, 2 at the poles and 4 at the equator. The 4 is a split of the 8, a regular number and equidistant. The 3 are around the equator at 120 degrees asunder; the 2 at opposite poles.²¹

These new tools were the size of gumballs and were drilled with varying numbers of holes that enabled the spheres to be connected by pins. In a number of the balls, the holes were equidistant to reflect the notion of simplicity and most likely association. The use of such three-dimensional, tactile tools meant that Dalton and his students had a better understanding of the actual molecule, demonstrating a stereochemical perspective. This has led to authorities such as Rouvray calling Dalton 'the world's first stereochemist'.²² Despite this claim, he was not the only early chemical atomist to engage in stereochemical thinking, as William Wollaston also recognized three-dimensions and produced wooden models to illustrate his ideas.

²¹ Dalton, 1840-1842, 41-42.

²² Rouvray, 1995, 52.

Dalton's system of modelling

Having previously discussed Dalton's symbols as a system of representation and a visual, 'paper' tool, it is prudent to address his three-dimensional models in a similar manner. The notion of a scientific tool is a concept that historians of science have discussed for many years; most have an open mind when it comes to what counts as a scientific tool.²³ While 'tool' often infers something tangible, as Dalton's wooden balls were, the word has been redefined in terms of function. Tools assist in investigatory science and scientific education. The most useful tools from the history of science include the balance and the microscope.²⁴ These can be considered more laboratory equipment as they are fundamental to investigation, whereas I view a tool as something more supportive and descriptive. In this vein, Dalton's wooden balls were useful musing and pedagogic aids that helped him to visualize his two-dimensional construction. In this part of the paper I will examine the design and implementation of Dalton's wooden balls, paying particular attention to their stereochemical properties.

The nature of Dalton's atomic models

Atomic models are useful tools for visualizing the structures and shapes of groups of atoms, which is important for understanding their behaviour. Modelling is an important aspect of modern chemistry. Dalton was one of the first people to use ball and spoke models to represent the structure of molecules.

²³ Gass, 2007, 350.

²⁴ Gass, 2007, 350.

Some of Dalton's atomic models survive and provide an intriguing insight into pedagogical tools from the early nineteenth century.²⁵ There are two known sets of Dalton's atomic models: one in the Science Museum in London and the second in the Museum of Science and Industry in Manchester (MOSI).

Looking at the balls in detail, the models from the Science Museum appear to have traces of coloured paint on them, to denote the different atoms. This colouring is common in today's Molymod kits, but could be unusual and innovate for the time. I suggest that the models were originally coloured black, white and brown. The models from the Science Museum seem to correspond with the ball with twelve equidistant holes and the one with two at opposite poles.

The second set, from MOSI (see Figure 6), is more interesting as they represent atoms of different sizes. The models are graduated and could easily be used to represent compound atoms (molecules) such as hydrate of potash, which Dalton depicted as having one larger and two smaller components. Despite having the models created in 1810 and using them in his lectures and for other demonstrations, he failed to publish details of them until 1842, two years before his death. Thus, many of Dalton's conjectures on the spatial positions of atoms in molecules were published after his death by Roscoe and Harden in their work of 1896.

²⁵ Gass, 2007, 365.



Figure 6: Set of atomic models from MOSI (author's own image). The British 2p coin is given for size comparison.

Dalton and stereochemistry

Stereochemistry refers to the study of the relative spatial arrangement of atoms within molecules. The prefix 'stereo' denotes the three-dimensionality of the molecular models. The emergence of stereochemistry is usually associated with the second half of the nineteenth century and the work of Jacobus Van't Hoff.²⁶ Until the early 1870s chemists lacked the conceptual tools to picture and model three-dimensional molecules.²⁷ Even apparently structural formulae indicated only the arrangement of atoms, links in a chain rather than positions in space. Historian of chemistry Trevor Levere noted that it would be difficult to know the real positions of atoms in space.²⁸ This

²⁶ For a more detailed analysis of the history of stereochemistry see Peter J. Ramberg *Chemical Structure, Spatial Arrangement: The Early History of Stereochemistry, 1874-1914.*

²⁷ Levere quoted in Ramberg, 2005, xxi.

²⁸ Levere quoted in Ramberg, 2005, xxi.

is true, and while many of Dalton's arrangements are incorrect or highly unlikely (such as a dodecahedral molecule) others are related to modern molecular models. The importance of stereochemistry was not fully recognised in the early nineteenth century and as such the majority of Dalton's models are basically topological.

Looking at Dalton's compound atoms, those he termed binary and ternary are linear and as such have predicted bond angles of 180°. These can be easily modelled using Dalton's balls. Molecules such as sulphurous acid (one azote and three oxygen according to Dalton) were drawn with one central atom of azote and three outer atoms of oxygen arranged equidistant as if on the corners of an equilateral triangle. This trigonal arrangement is evident from the existing atomic models and Dalton's own admission of having a ball with three holes "around the equator at 120 degrees". The simplicity of the linear and trigonal arrangements reflects the assumptions he made when combining atoms.

Given Dalton's specifications there was scope to create various molecular models using the balls with twelve and eight equidistant holes. These balls could be used as a central atom and enabled Dalton to vary the number of connections. As they had holes across the entire curved surface and not just around the equator, it suggests arrangements away from the planar (such as the aforementioned linear and trigonal). This move towards the tetrahedral and octahedral is reinforced by a drawing in Dalton's own notebook from March 1834. Figure 6 depicts a three-dimensional tetrahedral arrangement for the oxamide molecule in Dalton's own hand. The formulae for the molecule demonstrate that he believed the compound was composed of one atom of carbon (shaded circle), one atom of hydrogen (circle with a dot), one atom of nitrogen (circle with vertical line), and one atom of oxygen (open circle). Dalton appears to be attempting to depict stereoisomers of the oxamide molecule.²⁹ The placement differs from versions of four-atomed compounds in *A New System*, as the central (fourth) atom is drawn overlapping a triangular arrangement of the other three. This layering is unusual in Dalton's work, but there is the possibility that the quaternary elements (compounds) in Figure 2 were in fact two-dimensional representations of tetrahedral molecules. If this is indeed the case, it raises questions about the intended threedimensional arrangements of the other compounds listed in Figures 2 and 3. Currently this is speculation, but the intricacies of producing a printed plate depicting tetrahedral (or other three-dimensional arrangements) would create problems for the printer and therefore financial considerations for the publisher.



Figure 7: Three-dimensional representation for the oxamide molecule (from Dalton's notebook, No. 11, March 1834, p. 372 reproduced in facsimile by Coward, 1927, p. 34).

An interesting comment from Dalton was that seven atoms were "an awkward number to arrange around one atom" suggesting that he thought in terms of both simplicity and design.³⁰ Certainly, an aesthetic consideration could point towards his belief that his system of notation was "the only one representing nature" and nature was inherently symmetrical and pleasing to the eye.³¹

²⁹ Coward, 1927, 34.

³⁰ Dalton, 1840-42, 42.

³¹ Thackray, 1972, 118.

What could a three-dimensional model offer Dalton?

Dalton used his two-dimensional symbols in both his research and teaching. They were reproduced in *A New System of Chemical Philosophy* and also found their way into his correspondence (Figure 8). Thus, they were a useful paper tool and part of a visual language. In terms of his models, the question that we must ask is: can a system of notation such as Dalton's atomic symbols be transformed into a tactile, user-friendly system? It seems evident that this was one of his aims with respect to creating the wooden models as their design correlates to the two-dimensional paper versions of compound atoms. The set of graduated models demonstrated this most effectively as they could have been manipulated to represent a plethora of designs. But the question remains as to whether it was a user-friendly and indeed, useful system.

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Figure 8: Letter from J. Dalton to J. L. Gay-Lussac (5 August 1833): use of an encompassing circle to (possibly) separate compound atoms (author's own image of MM/1/7 from The Royal Society archives).

Modelling molecules is an important part of modern chemistry teaching, however, the reasons behind the use of models has changed over the past two centuries. Transforming a collection of balls and spokes into a three-dimensional representation of an atom, then combining two or more into a compound demonstrates a chemical process, which can be considered a chemical language. Combining actual chemicals in the laboratory and seeing the reaction is visually rewarding, particularly if an effervescent or explosive reaction is seen, so it is sensible to use a visual language to theoretically represent such a process. Being able to handle and manipulate molecules could also aid retention among his pupils, thus their use as a teaching aid was not only connected with the scientific but also the kinesthetic.

Conclusions

The focus of this paper was Dalton's visualisation of chemical elements and their bonding; Dalton used both pictorial and alphabetical notion to create his symbols within circles, representative of his concept of the atom. Although not conducive to classification, it is interesting to note that when students draw representations of atoms and bonding at school nowadays they initially draw a circle to represent the atom, as Dalton had done two centuries earlier, before attaching the relevant number of electrons.

It has been said that, "Symbolic formulae ... would deserve to rank among the chemist's most powerful instruments of research."³² I would expand this idea to include all chemical symbols and not just limit their use to an instrument of research, but as a useful tool for teaching and learning. Through his use and manipulation of symbols

³² Hofmann, 1865, 87.

and 3D models it suggests his deductive reasoning and visual thinking.

By creating three-dimensional representations of his atomic symbols, Dalton was able to investigate the composition and structural arrangement of molecules. It is clear from other studies that stereochemistry was very much an emerging discipline in the nineteenth century, so Dalton would not have fully understood the implications of the models. However, the ball and spoke system is simple and by virtue of its application to chemical problems suggests deductive reasoning and visual thinking on behalf of Dalton and his pupils. As a modelling system, it perhaps did not achieve its full potential in the hands of Dalton, but its descendants are seen in the schoolrooms of today. As a pedagogic tool and a physical *aide memoire* the balls could be deemed useful but further investigation is necessary to prove this beyond mere conjecture.

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