

Ampère and the "Representative Shape" of Molecules

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INTRODUCTION

The history of science is more than just a retelling, more or less of the same thing and contextualised in a given time. It is re-reading. Evolutions, continuities and affiliations are just as important as the reconstruction of what is expressed in a more or less distant past.

So, the present article returns stereochemistry history to the *longue durée*, consisting of three parts. Firstly, I draw attention to Wollaston's and Ampère's contributions, as well as the likely reasons for their lack of public impact. I will then focus on Ampère's only publication, defining molecular structure for the first time, before being described as polyhedral. This gave substance to the notions of the crystallographer René-Just Haüy (1743-1822), who had already advocated a geometric approach to the structure of molecules (using modern terms). This geometric vision is part of a Pythagorean mentality, creating a link among scholars, occasionally separated by centuries but united by a common intuition on the importance of Platonic solids, from Kepler and Robert Hooke to Alfred Werner¹. Most of them also shared their desire to base chemical structure on Descartes's incisive mathematical physics. I will conclude by denouncing that stereochemistry emerged in 1874, from the announcement of the tetrahedral carbon atom by Achille Le Bel and Jacobus Henricus van't Hoff². This sub-discipline is actually much older.

Essentially, my analysis is on Ampère's publication in *Annales de Physique et de Chimie* in 1814.

1. Alfred Werner (1866-1919), Swiss chemist, Nobel Prize in Chemistry in 1913 for his explanation of the structure of certain metals.

2. Achille Le Bel (1847-1930) and Jacobus Henricus van't Hoff (1852-1911, first Nobel Prize in Chemistry in 1901) worked together in Paris in Adolphe Wurtz's chemistry laboratory during their studies.

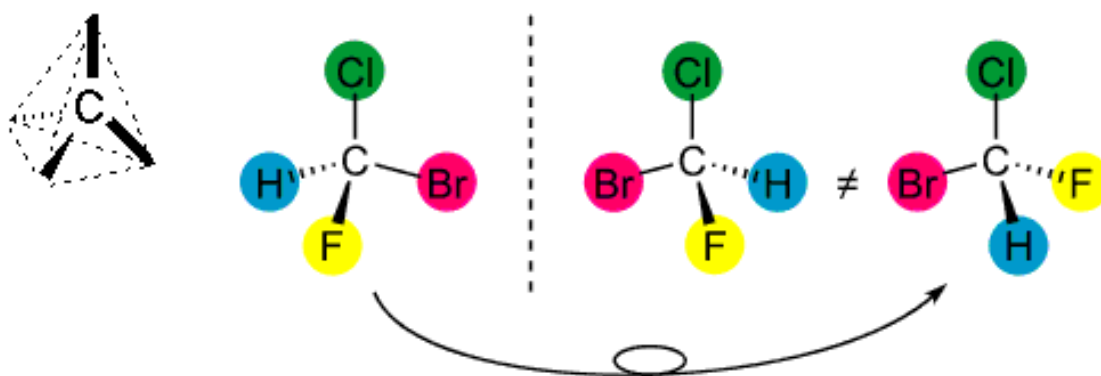


Figure 1: Importance of spatial configuration (stereochemistry): the case of chirality³. On the left, in black, the "tetrahedral" carbon atom: it can be linked to four atoms at the vertices of a tetrahedron of which it is the centre. Such distribution in the space of different atoms - for example around a point (C in the middle) - leads to non-stackable configurations in a mirror, thus different chemical objects. In colours, the two molecules (separated by a dash which symbolises the outline of a mirror) are mirror images: if we turn the first (which leads to the third, on the right), we see it is not superimposed on the second, in the middle. It consists of a different chemical compound: the initial molecule known as chiral: it is not superimposable on its own image in a mirror.

WOLLASTON'S BAKERIAN CONFERENCE

William Hyde Wollaston (1755-1828), a native of Dereham, Norfolk, is best known for his production of platinum using a process that he kept confidential and which proved highly lucrative, firstly working with Smithson Tennant (1761-1815), and then, from 1805, with William Cary (1759-1825). But he had many other interests, crystallography among others. He perfected the goniometer that René-Just Haüy had designed for measuring angles of crystal faces. In 1809, he published his design of a reflecting goniometer in the *Philosophical Transactions*. He was therefore familiar with Haüy's work and ideas. In addition, he was interested in atomic theory, both criticising and modifying John Dalton's ideas.

3. On the property of chirality and the optical rotation of molecules, as analysed by Fresnel in 1822, see Bib-Num [analysis](#) carried out by Jeanne Crassous.



Figure 2: Father René-Just Haüy, inventor of crystallography. He was the brother of Valentin Haüy (1745-1822), founder of the first school for the blind.

These concerns are found in the *Bakerian Lecture* that he gave in 1812 at the Royal Society, published in 1813. Wollaston took as his starting point Robert Hooke's comment in his *Micrographia* on the construction of geometric solids such as the tetrahedron from spherical particles. Yet, Wollaston is uncertain: should he choose the tetrahedron or the octahedron as a basic module in crystallography? The rhombohedral shape of the Iceland spar also fascinates him. He shows his audience how we obtain, while assembling spherical objects, at choice, a tetrahedron, an octahedron, a rhombohedron, a hexagonal prism, etc.

Incidentally, he describes what we know now as the crystal structure of sodium chloride, a cubic structure alternating two types of particles. I will quote here just one more passage from this conference, for clarity:

And though the existence of ultimate physical atoms absolutely indivisible may require demonstration, their existence is by no means necessary to any hypothesis here advanced, which requires merely mathematical points endued with powers of attraction and repulsion equally on all sides, so that their extent is virtually spherical, for from the union of such particles the same solids will result as from the combination of spheres impenetrably hard.

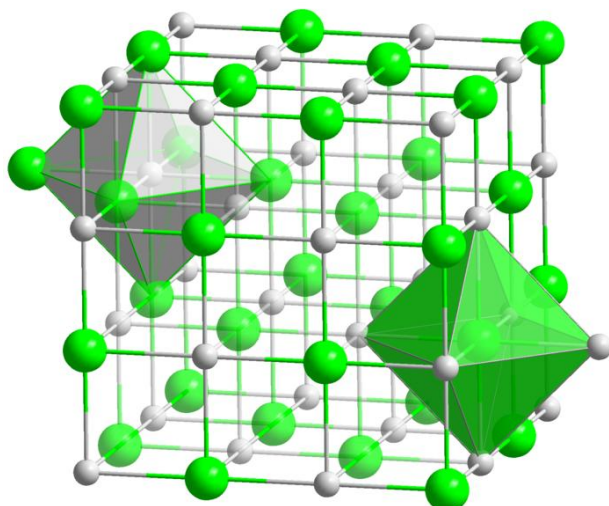


Figure 3: Diagram of the crystal structure of NaCl (sodium chloride). It's a network known as "face-centred cubic" where chlorine ions (in green) occupy a cube's vertices, and sodium ions (in grey) occupy the centres of this cube's edges, or vice-versa. We also note that sodium ions are distributed in octahedra around each chlorine ion (green octahedron on the right) (image Wikimedia Commons, Solid state)

AMPÈRE'S ARTICLE

In 1814, the year following Wollaston's publication, a *Letter* was published from Monsieur Ampère to Count Berthollet about the determination of the proportions in which bodies combine, from the number and the relative disposition of the molecules from which their integral particles are composed. His contemporary chemists hardly paid it much attention, explaining how this brilliant article simply disappeared. Perhaps Ampère was not a chemist, but he was undoubtedly a major figure in chemistry. Likewise, he tried his hand at a systematic classification of elements in families, therefore anticipating Mendeleev's for decades.

In this 1814 article, Ampère poses the existence of molecules in three-dimensional space. If each atom occupies a polyhedron's vertex, then this polyhedron will serve as the representative shape of the molecule:

...a polyhedron in which each molecule occupies a vertex, and it will suffice to name this polyhedron for expressing the relative situation of the molecules in which a particle is composed. I will give this polyhedron the name representative form of the particle⁴.

4. We should always be vigilant when reading Ampère: he refers to molecule (now called atom), and particle (now called molecule).

On the other hand, due to the gas laws established by Joseph Louis Gay-Lussac (1778-1850), the relative numbers of atoms in a molecule is deduced from the volumes of gas. Ampère relates the following approach of his to Gay-Lussac's and Avogadro's, mentioning both⁵:

I left, for this, on the assumption that, in the case where the bodies become a gas, their only particles [molecules] are separated and spaced from one another by the expansive force of heat, at distances much greater than those where the forces of affinity and cohesion [the forces of attraction between atoms of a molecule] have an appreciable action, so that these distances depend only on the temperature and pressure that the gas supports, and that at equal pressures and temperatures, the particles of all gases, either simple, or compound, are equally distanced from each other. The number of particles is, in this assumption, proportional to the volume of gas.

[...]

water vapour containing, from Monsieur Gay-Lussac's beautiful experiments, an equal volume of hydrogen, and half its volume oxygen, one of its particles [the water molecule] will consist of an entire hydrogen particle [a hydrogen molecule, or two hydrogen atoms], and half of an oxygen particle [or an oxygen atom]

Ampère distinguished five base modules for molecular geometry: tetrahedron, octahedron, parallelepiped, hexagonal prism and rhombohedral dodecahedron. He sees chemical combination as the congruent assembly of two polyhedra, each being the representative shape of molecules while uniting. A logical consequence of this theory is the possibility of deducing the elemental composition of such geometric considerations; Ampère provides some examples of them.

Ampère's Examples on Molecular Structure

The first construction given by Ampère is (p.12) a parallelepiped with two tetrahedra. There are two stages: in the first stage, Ampère takes (bottom of p.11) two equal and perpendicular lines forming a cross, in a plane. He then separates them by a certain distance, and "while always keeping them in a situation parallel to what they had in this plane", he obtains a regular tetrahedron.

5. See the corresponding BibNum dossiers: the article of Gay-Lussac (1809) [analysed](#) by Pierre Radvanyi, and of Avogadro (1811) by [Bernard Fernandez](#).

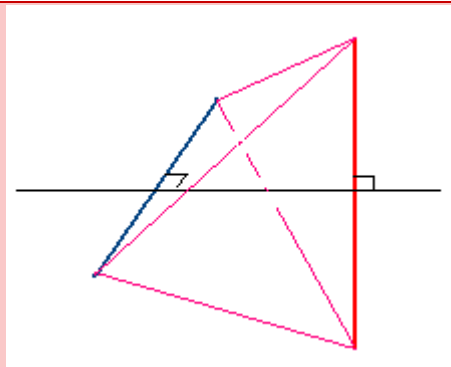


Figure 4: Construction of a tetrahedron from two straight lines, as indicated by Ampère. The view is here in perspective, in two perpendicular planes (red section and black line; blue section and black line). We removed the red and blue sections, originally perpendicular in the same plane (original situation not shown). Once these two sections are separated from their common centre, we join (in purple) one end of the red section to an end of the blue section, then the other. We obtain a tetrahedron, of four vertices (each end of the two sections) and four faces.

The second step is based on the first:

If we assume, in the case of the tetrahedron, carried out by the two lines which we have discussed, two mutually parallel planes, and that we place in each of them a line that represents the position where the line of another plane would be found before separating them, the ends of these two new lines will be the four vertices of a symmetrical tetrahedron (...), and the eight vertices of these two tetrahedrons, united in this way, will be those of a parallelepiped. The parallelepiped shape therefore results in the union of two tetrahedra.

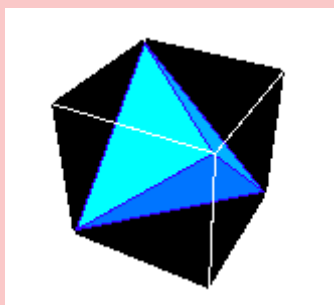


Figure 5: Construction of a cube from two tetrahedra, as indicated by Ampère. Here we have only represented a tetrahedron – incidentally, the situation in figure 2 is clear, with a top section (the diagonal of the top face of the cube), equivalent to one of the two sections of figure 2, and a bottom section (the diagonal of the bottom face of the cube), equivalent to the other section. In the sentence above, Ampère proposes to build a second tetrahedron (not shown) from the other diagonal of the upper face, and the other diagonal of the bottom face. The two tetrahedra combined make up eight vertices, those of the cube (image Académie de Nouméa).

Ampère makes certain deductions on the shapes of molecules. He takes the example of a body A, "whose particles [*molecules*] have for their representative shape a tetrahedron", and a body B, represented

by an octahedron. He tries to geometrically combine tetrahedra and octahedra in various proportions, in order to obtain polyhedra:

If we try, for example to combine tetrahedra and octahedra, so that the number of the former are half the latter, we only find bizarre shapes that have no regularity (...) We must therefore conclude [that bodies A and B] will not come together in a way that in the combination there is one proportion of A and two of B; on the contrary, this combination will be easy between two proportions of A and one of B, since two tetrahedra and one octahedron form, by coming together, a dodecahedron.

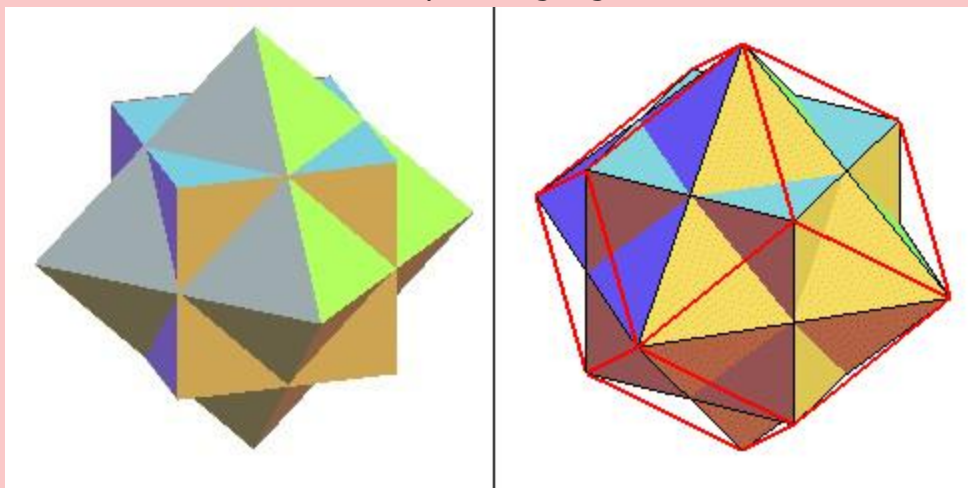


Figure 6: Construction of a rhombic dodecahedron from two tetrahedra and an octahedron, as indicated by Ampère. We saw that two overlapping tetrahedra form a cube (figure 5). We now overlap an octahedron in the formed cube (on the left). We connect in red lines the envelope of vertices (on the right): so, we obtain a polyhedron with 12 diamond faces and 14 vertices (the cube's six vertices and the tetrahedron's eight). The semi-regular polyhedron obtained is the dodecahedron (12 faces) known as rhombic, with diamond-shaped faces - not to be confused with regular dodecahedron, a Platonic solid, with pentagonal faces⁶ (images site Mathcurve)

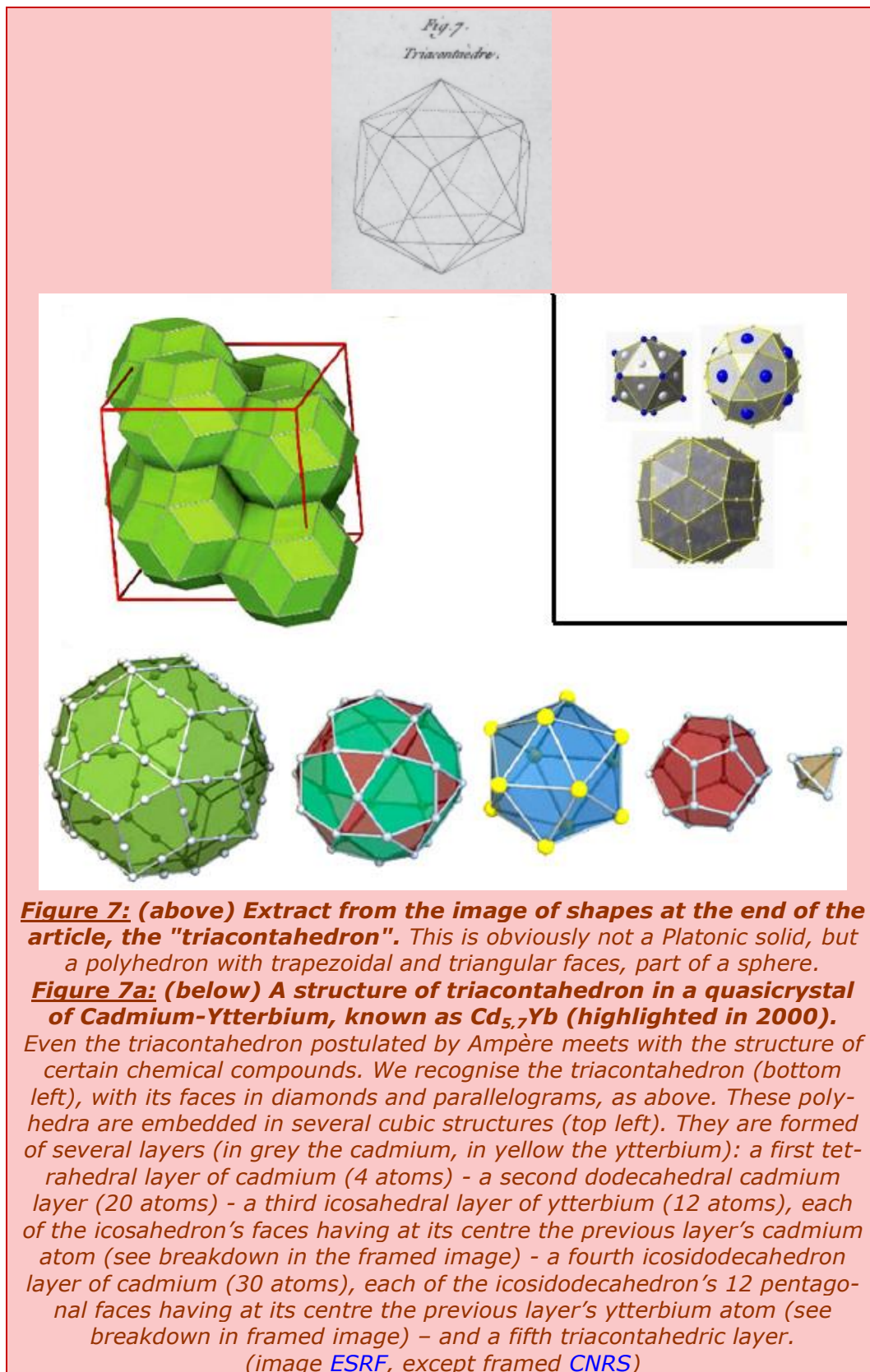
In the impossible case of geometric combination in polyhedron, Ampère hammers home the point:

These forms must be rejected; indeed, we observe that proportions that they would assume in chemical combinations do not meet in nature.

But the combination of A and B, "two proportions of A and one of B", is not the sole possibility. Ampère indicates a possible combination with equal proportions, and with two possible constructions (p.16):

- Combining a tetrahedron and octahedron into a "hexadecaedron", shown by Ampère.
- Combining two octahedra and two tetrahedra into a "triacontaedron", shown by Ampère.

6. Ampère does not give this precision, but figure 5's first image at the end of his article clearly shows that he talks about *rhombic* dodecahedron..



Ampère was well aware of the importance of his deductions. His introduction and conclusion are significant in this regard (conclusion p.39-40):

The results that I have just pointed out are only a very small part of those that can be deduced from the consideration of representative shapes of the body particles, applied to the determination of the proportions of inorganic compounds. The chemistry of [organic] organised bodies also provides many applications of this theory (...) I have drawn from it (...) several determinations regarding the composition of different substances taken from the plant kingdom, which agree too well with the experiment results to allow doubts on utility of which it may be in this part of chemistry.

In fact, Ampère later considers his contributions to chemistry as the very best of his scientific work⁷. The modern commentator has no reason to doubt it.

Ampère was building on solid foundations, of two types. Gay-Lussac had found that gases combine following simple numerical ratios. René-Just Haüy, who had the idea to shatter a calcite crystal, discovered that a crystal's unit cell, in today's language, indefinitely reproduces by translation in each of the three dimensions. Thus, the geometric shape espoused by a real crystal, on the laboratory scale, informs us of the structure on a microscopic scale. Note that Haüy's intuition can be identified as *mise en abyme*, a figure of speech familiar to the writers of the seventeenth and eighteenth centuries.

Ampère's article is explicitly set in the movement of Haüy's ideas. For the latter, the *integral molecule*, the concept that Haüy introduced since 1784 in his *Essay of a theory on the structure of crystals*, should be a tiny polyhedron, since the macroscopic shape of a crystal only enlarged the microscopic modules within it. A crystal's cleavage, whether real or a thought process, would reveal the primitive form that it shares with a whole family of related minerals: we cannot help but think of the Platonic archetypes. Ampère was not satisfied by taking over this concept of integral molecule, which he renames "particle". Additionally, he borrows five of Haüy's six primitive forms, with the exception of the dodecahedron with triangular isosceles faces. Ampère stands out slightly from Haüy when he identifies integral molecules and primitive forms.

What did Haüy make of it? In 1814, he had conserved all his mental agility: proven in the following year, he formulated his law of symmetry, and therefore

7. In a letter dated 11th March 1914 to his friend Roux, Ampère mentions as follows the combination law of chemical bodies proposed in his article: "a law of nature whose discovery may be, after what I did last summer in metaphysics, the most important thing that I will have developed in all my life" (quoted by Michelle Sadoun-Goupil, "Esquisse de l'œuvre d'Ampère en chimie", *Revue d'histoire des sciences*, 1977, **30**, no. 30-2, pp. 125-141 (online at Perseus)).

bringing his work on crystallography to a close. There is no doubt that Wollaston's and Ampère's articles were pointed out to him.

Their contemporaries clearly saw the narrowness of the reports. The most incisive evaluation was, in a somewhat unexpected manner, by the literary critic Saint-Beuve (1804-1869) who wrote in 1843:

"Monsieur Gay-Lussac's discovery of simple proportions observed between the volumes of a compound gas and those of component gases became for him [Ampère] a means for conceiving, about the atomic and molecular structure of inorganic bodies, a theory which replaces Wollaston's"⁸.

Furthermore, this may well be the very first use of the expression "atomic and molecular structure"!

Meanwhile, Ampère introduced the expression *forme représentative*. This is of great interest, because it seems over the top. Its use suggests that Ampère from 1814 led an epistemological reflection, of the kind that would fully mobilise it from 1828. If it were attached to the *particle form*, i.e., a molecular property (using our current terminology), then we would have been able to accuse it of having no effect on a scientific hypothesis of pure and simple speculation. Yet, having the ability to use the expression *representative form of a particle*, Ampère put emphasis on what were the polyhedral shapes that he conjectured of mind over matter projected properties, rather than of intrinsic qualities. This representative form was inherent to the description, not necessarily to the described object. Here is what this apparent tautology implies of representative form. In other words, this 1814 article is written from a cryptoristic, not cryptological, point of view, using Ampère's vocabulary in *Classification of sciences*: to discover something hidden, rather than elucidate the causes of the observed facts.

Ampère's article is important for its generalisation of Haüy's ideas from mineralogy to chemical compounds in their entirety. It also includes a fundamental intuition, with programmatic value unfortunately not perceived during the nineteenth century, whereby elemental composition is derived from molecular structure; therefore, chemical analysis could not precede, but follow structural determination. Ampère even publishes a table of correspondence. He says:

8. Charles-Augustin Sainte-Beuve. "Notice sur M. Ampère", In : André-Marie Ampère, *Essai sur la philosophie des sciences*, t. II, Paris, 1843, p. I-LIX (en ligne sur Gallica).

the consideration of representative forms foreshadows (...) how much, in a composed body, it must enter from molecules [read: atoms] of each of its elements.

THE SMALL IMPACT OF AMPÈRE'S ARTICLE

This great article fell into a void. As we know, the Avodagro-Ampère hypothesis was ignored until Stanislao Cannizzaro resurrected it at the Karlsruhe Congress in 1860. Was it a premature discovery? John H. Brooke responded to it negatively, after having produced a dozen hypotheses about the reason for the half-century delay between the Avogadro's publication and the Karlsruhe Congress. His argument is generalizable to Wollaston's and Ampère's theories.

There were two reasons for the rejection of Ampère's ideas, both of which are explicit. They were speculative, worse still they were the work of a physicist. As expressed by Jean-Baptiste Dumas (Lessons of chemical philosophy, 1836):

Ampère's hypothesis, no matter how ingenious it is, is absolutely unacceptable. Such is the fate, and this circumstance is to be noted, as is the fate of affinity systems and molecular group systems presented by physicists. Even when they have, like Monsieur Ampère, exact notions on phenomena and laws of chemistry, the usual lack of practice of this science is always felt at home.

What happened between 1814, the date of Ampère's letter to Berthollet, and 1836, when Dumas rejected Ampère's theorisation? An entire generation of chemists had the opportunity to study Ampère's geometric notions applied molecular shapes. Altogether, they rejected them. But why was this?

Besides the reasons presented by Brooke in the case of Avogadro, I see four of them. By ordering them by increasing importance, 1st – due to the state of scientific publications in Europe at the start of the early nineteenth century, Avogadro's and Ampère's contributions came in a dispersed order; moreover, they largely ignored each other; if they had been able to stand together, this could have changed the table; 2nd - these contributions were not considered useful or applicable, they also suffered from inconsistencies, both internal and external (with John Dalton's atomic theory); 3rd - they were part of the Newtonian mathematical physics program, that the scientific and political demise of the Society of Arcueil (with Louis XVII's restoration) had condemned in France; 4th -

effectively, these three contributions had frightening traces of mathematical physics: they tended to erase the gap between chemistry and physics, just as these two disciplines began their professionalisation.

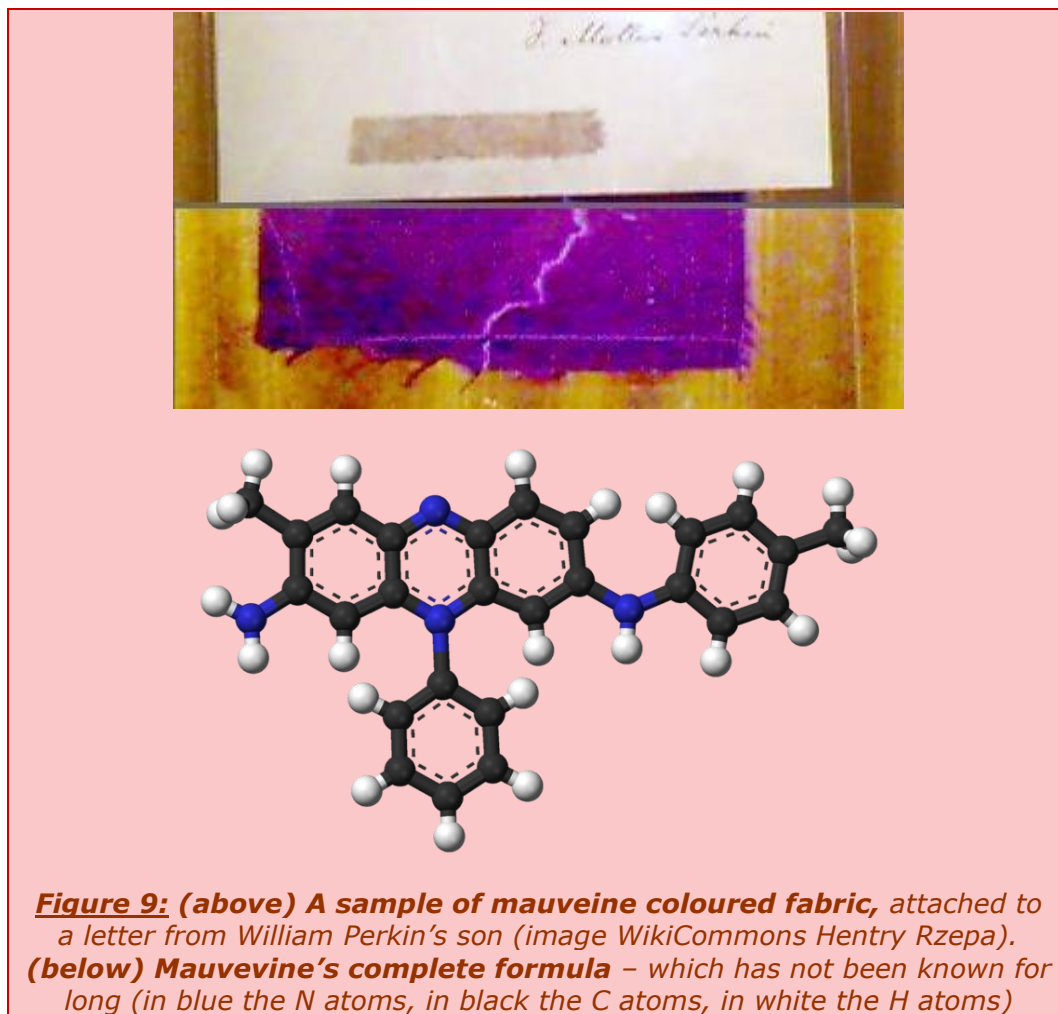
Nonetheless, some young chemists took Ampère's ideas seriously. This was the case for Marc-Antoine Gaudin (1804-1880). Having attended Ampère's classes, he converted his own ideas. Consequently, he decided to dedicate himself to the description of molecular shapes, and to deduce the molecular architecture of crystal structure. His contributions were not even rejected, but remained ignored the whole time. Nobody took him seriously. He was not part of the established system; he was a lightweight, insignificant. Alexandre-Édouard Baudrimont (1806-1880) was a realist in the same vein as Ampère, as well as an antipositivist. This scientist, in Ampère's intellectual movement, fought in vain for structural chemistry over reactivity studies. Additionally, he was kept away from mainstream French chemistry, 1830-1880. Doctor and pharmacist in training, he was appointed to a chair of chemistry in Bordeaux in 1849. Consequently, he was forced to limited influence.

THE RETURN OF THE REPRESSED

As late as 1856, the young William Henry Perkin (1838-1907) remained sufficiently convinced of what was the elemental composition in biunivocal correspondence with molecular structure, to attempt a synthesis of quinine ($C_{20}H_{24}N_2O_2$) by simple doubling of allyltoluidine ($C_{10}H_{13}N$); this led him to the unexpected discovery of a new dye, mauveine.

Mauveine, the First "Industrial" Dye

In 1856, by an artefact, Perkin, cleaning the container with residues of his failed synthesis of quinine test, noticed that some of them are soluble in alcohol, forming a purple solution. The first industrial dye for colouring silk and fabric was born - a factory for the manufacturing of mauveine was built in Greenford, west London. Industrial synthetic dyes replaced progressively natural coloured pigments.



This episode has two lessons. In 1856, the analysis of organic molecules for determining composition was already practiced vigorously for a good generation. Justus von Liebig (1803-1873), in his laboratory in Giessen, under profound and lasting influence, as a model across Europe, trained there young chemists from 1824 to 1852. Such elemental analysis was the basis for this training.

Chemists of this time characterised the substances they isolated by their composition, which completed the melting point, boiling point and other physical constants. The synthesis attempt of quinine by Perkin, who from our perspective appears very naive, clearly shows how far, on the very eve of structural chemistry development in the wake of the Karlsruhe Congress (1860), determination of elemental composition took precedence over all other considerations.

However, chemists had hardly realised the huge proliferation of organic chemistry molecules. Perkin's great blunder begins with a collective mentality by

not measuring all consequences of Isomerism, of how extravagant molecules are by sharing a common composition. Yet, this phenomenon had been discovered 30 years earlier by Liebig and Friedrich Wöhler (1800-1882), receiving its name from Berzelius in 1830-31. Chemists accepted it reluctantly; yet, this did not prevent them from remaining confident that elemental composition served as any molecule's sufficient and complete signature.

Where did their blinders come from? Throughout the first half of the nineteenth century, chemistry was underpinned by a research program aimed at developing classifications of chemical compounds on the model of different systematics of biological organisms. Chemists of this period targeted a classificatory scheme on two terms, similar to the Linnean classification, wherein one word defines the genus and the other the species. This mentality was anchored in the chemical analysis, a strict routine using the tool invented by Liebig, his *kaliapparat*. The beginnings of the chemistry professionalisation that intervened at the same period, and then the industrialisation of dye chemistry that followed Perkin's discovery, only served to conclude this simplistic notion of a biunivocal correspondence of an elementary formula and molecule.

As we know only too well, changing a mentality is extremely difficult. Only snipers would try it. This was the case of two young chemists, a Frenchman, Auguste Laurent (1807-1853), the other British, Archibald Couper (1831-1892), who because of this had trouble with the establishment. It is only around the mid-1850s that this mentality, resistant to Ampère's ideas, began to evolve. The empirical collection of raw data, in the spirit of positivism, little by little gave way to an analysis, lexical and syntactic, of chemical formulas like words.

This mutation saw the introduction of new formulas, known as developed, bearing information on the connectivity of atoms in a molecule. This was a multiple discovery (science historian Sarton noted that most discoveries are simultaneously the fact of several people) attached to Couper (1858), Kekulé (from 1857), Loschmidt (1861), Crum Brown (1861), Wurtz (1864), Hofmann (1865) ...

Chemical science returned to hypothetical-deductive methodology, which Ampère had tried to guide. Regarding this, the example of Friedrich August Kekulé (1829-1896) and his intellectual development is the most telling. In 1858, he was still holding for equivalents a "rational formula" and *Umsetzungformeln*,

i.e., a kind of shorthand for all observed facts, relating to transformations that a given compound had undergone. In 1866, with his cyclic formula of benzene, Kekulé had completed a *Gestalt* turnaround. The formula, hexagonal or triangular (depending on whether we believe Kekulé's formula or alternatives proposed by his contemporaries) - returning to Ampère's geometric shapes - had become an a priori intellectual construction: as a hypothesis to confront experimental data.

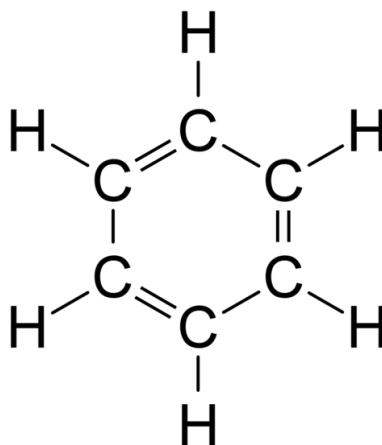


Figure 10: Benzene's developed formula C_6H_6 . This hexagonal representative shape, with double Carbon bonds, demonstrated around 1864 by August Kekulé von Stradonitz (1829-1896) (image WikiCommons Leyo).

THE HISTORY OF STEREOCHEMISTRY AND THE LONGUE DURÉE

To begin with, note that the two terms "stereoisomer" and "stereochemistry" date back to 1888. These names are indicators, rather than some opening of a new disciplinary field, of its adult age. Generally, disciplines and sub-disciplines adopt an organisation, name, terminology, specialised journal and training programme for young researchers, after the initial push (the development of instruments and procedures, the establishment of concepts) has already developed into such institutionalisation.

So, if we pose that stereochemistry, as a conception, had reached maturity in the 1880s, when did it begin? Various historical accounts differ on this point. We find two main schools. One chooses the date 1874 which saw announcements of the tetrahedron carbon, almost simultaneously by Le Bel and van't

Hoff. Other authors choose the year 1847, and Pasteur's early work on tartaric acids. This difference is almost 30 years – the duration of a generation.

Anyway, whether you choose one date or the other, the decision is undermined by the existence of an entire prehistory to stereochemistry. In the first case, is it not clear that van't Hoff found the idea of a three-dimensional representation (for tetrahedron carbon) in Kekulé's laboratory in Bonn, where he stayed in 1872-73? Was Kekulé himself not influenced by Butlerov's guesswork in 1862, following which carbon affinities spread tetrahedron carbon vertices? Van't Hoff's tetrahedral hypothesis, as he admitted himself, had yet as another source the study of lactic acids in 1869 by Johannes Wislicenus. This concludes that an isomerism comes from the different spatial arrangement of atoms. In 1873, Wislicenus wrote about this subject:

if molecules can be structurally identical and yet possess dissimilar properties, this difference can be explained only on the ground that it is due to a different arrangement of atoms in space.

How Achille Le Bel benefited from Pasteur's ideas is equally obvious. Pasteur himself did not just innovate from nothing. His separation of right and left isomers of tartaric acids was not an ex-nihilo innovation. He was indebted to Auguste Laurent for it, who had suggested to him to study crystals of tartrates for his doctoral work.

These indications will be enough to convince us of the frivolity that there would be to dismiss the stereochemistry of 1874, or even 1847. In my view, the only perspective to replace stereochemistry history can only be the Braudelian *longue durée*: "a history whose passage is almost imperceptible, that of man in his relationship to the environment; a history in which all change is slow, a history of constant repetition, ever-recurring cycles", one "almost outside of time".

What would stereochemistry history be like, written in the *longue durée*? It is intimately linked, to all stages, to the development of crystallography and, therefore, it goes back to at least the Renaissance.

Pythagorean beliefs in numerology were written in the sky when Kepler's neo-Platonic mysticism prompted him to inscribe the planetary orbits in Platonic polyhedra. He had this idea in 1595. It permitted him, in 1618, to formulate his third law, considered harmonic, to describe the solar system. Are we very far

from molecular shapes? Surely not, since the same Kepler (*Strena sive de nive sexangula*) realised, in 1609, symmetry of order 6 of ice crystals by the stacking up of little elementary droplets of constituent water. There was then a very early stage in history of molecular geometry, and therefore stereochemistry too.

During the seventeenth century, Kepler's intuition was taken up and developed by Descartes, Bartolin, Boyle, Hooke and Huygens. Robert Hooke, for example, showed the invariance of the angles of faces in a crystal independently of its size. While Kepler had seen Platonic solids in various ores, Steno abandoned Platonic solids for exact measurements of hematite crystals coming from the island Elba. A century of observations accumulated, until Haüy formulated his reticular hypothesis in 1802. In addition, and to return to the snowflakes that Kepler had scrutinised so closely, we are indebted to Haüy for having recognised that senary symmetry was only compatible with bent constituent particles (our molecules). For him, it was a visionary inference.

The second stage in the gradual *mise en abyme* of the material world was thus reached at the end of the eighteenth century when the same Haüy represented the shapes of crystals, basing them on regular polyhedra taken as basic blocks. The Platonic idea, inherited from the Renaissance, then came to encompass all mineralogy.

The third was the open letter from Ampère to Berthollet in 1814, to be discussed. From now on, we can describe - although few chemists ventured there - molecular structure by the atoms located at the vertices of regular polyhedra, in grateful arrangements of simple mathematical relations. Ampère was a pioneer, in that he pointed out notions of molecular structure and architecture as goals to achieve: for chemical science to establish and explain them; for chemists to use them to unravel the tangle of laws governing chemical combinations.

The fourth stage, if you believe me, an echo similar to Ampère's 1814 letter, is Auguste Laurent's thesis in 1837. This chemist, very informed in crystallography, familiar of René-Just Haüy's texts, wrote his thesis on the reactivity of organic molecules with respect to additions and substitutions. He designed a hydrocarbon nucleus, in the shape of a parallelepiped, having eight carbon atoms and twelve hydrogen. In doing so, Laurent conjectured a regular solid, a polyhedron which summarised and gathered all metamorphoses that an organic mole-

cule was likely to undergo. This was one of the seeds for Kekulé's 1859 conception of carbon tetravalence (the fifth stage).

The sixth, in this continuing *mise en abyme* throughout the ages, dignified although slow, was Le Bel's and van't Hoff's discovery in 1874: the tetrahedron, one of the five Platonic solids, proved to be a perfect descriptor of the tetravalence like the possible asymmetry of the carbon atom. During the 1890s, Alfred Werner made good use of the octahedron, another Platonic solid, as a template for the entire class of coordination complexes, or "higher order compounds", as he described them, and in order to demonstrate their isomers.

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Ampère's 1814 letter therefore bridges together Haüy and Werner. Werner's contribution put order in the proliferation of coordination compounds, organising them into three classes or family, of coordination numbers of four, six and eight. Regular polyhedra also appealed to him, in particular the octahedron for coordination six. Ampère's and Werner's contributions are both geometrically inspirational. The Nobel Prize was awarded to Alfred Werner in 1913. In his acceptance speech, Werner mentioned "the groups, potentially symmetrical, of four, six or eight points around a centre, where the adjacent points are equidistant", therefore giving a description of the coordination sphere around a central atom.



Figure 11: Alfred Werner (1866-1919), Nobel prize in Chemistry, 1913.

But that is not all, the *mise en abyme* outlined here was not interrupted with Werner's coordination theory. Then, at the start of the twentieth century, Gilbert N. Lewis was intrigued by the coexistence of two types of interaction of

interatomic bonding, the normal covalence in organic molecules and the dative bond in Werner's coordination complexes. This prompted him, from 28th March 1902, to represent electron configuration, at the back of an envelope, by yet another Platonic solid, the cube. In his scheme, the electrons formed a layer, gradually and symmetrically occupying a cube's vertices. In his own words, he convinced himself that,

the pair of electrons forms the stable group, and we may question whether in general the pair rather than the group of eight should not be regarded as the fundamental unit.

This gave him the notion of the two-electron chemical bond, and in this way it also demonstrated the tetrahedral carbon atom. Lewis was lead to conclude that the electrons were in pairs as if they were held together by small magnets; which anticipated the electron spin discovery and Pauli's principle. Here I see the eighth stage in what could be called **the platonisation of the material world**. This was also a major step in the reopening of a dialogue between chemists and physicists, during the first three decades of the twentieth century. It ended with the importation, for which we are indebted to Linus Pauling, of the main ideas of quantum mechanics; while physicists, such as Hans Bethe, Fritz London, Julius R. Oppenheimer, Edward Teller, and some others, who ventured into chemistry, retreated, discouraged by the complexity of this other discipline. Chadwick's discovery of the neutron was also available for many. They recovered physics with a charm thereby increasing to them. Both sciences then differed, chemistry giving predictive models, in a Fourier development, by acquiring information of inferior quality over an increasingly extensive domain. A physicist, however, aims typically at giving a predictive or interpretative capacity, in a Taylor series development, about a case-prototype like the hydrogen atom, by acquiring the best possible information, both on the prototype and neighbouring cases.

Moreover, the numerology underlying atomic and nuclear structures, that physicists like Elsasser and Geoppert-Mayer established during subsequent decades, still improved our knowledge of nature, from macrocosm to macrocosm, always on the basis of Pythagorean harmonies.

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Returning to the subject at hand, i.e., molecular formulas and the posterity of Ampère's letter, I will briefly mention (as latterly the gradual mise en abyme tirelessly unwinding since the time of Albrecht Dürer and Johannes Kepler) the heuristic announced in 1957 by several chemists under the name of *valence shell electron pair repulsion* (VSEPR or Gillespie-Nyholm theory); the reunification by Earl R. Muetterties in the 1960s, always in the spirit of Ampère, of organic and inorganic structures, whether aggregates of atoms, molecules or coordination complexes; Aaron Klug's discovery of the icosahedral viruses; the synthesis at the end of the twentieth century of isomorphous hydrocarbons of Platonic solids (Philip E. Eaton for the cube; Leo Paquette for dodecahedrane); and the fortuitous discovery (Richard Smalley, Harold Kroto and Robert Curl) of fullerene C₆₀, with truncated icosahedron geometry.

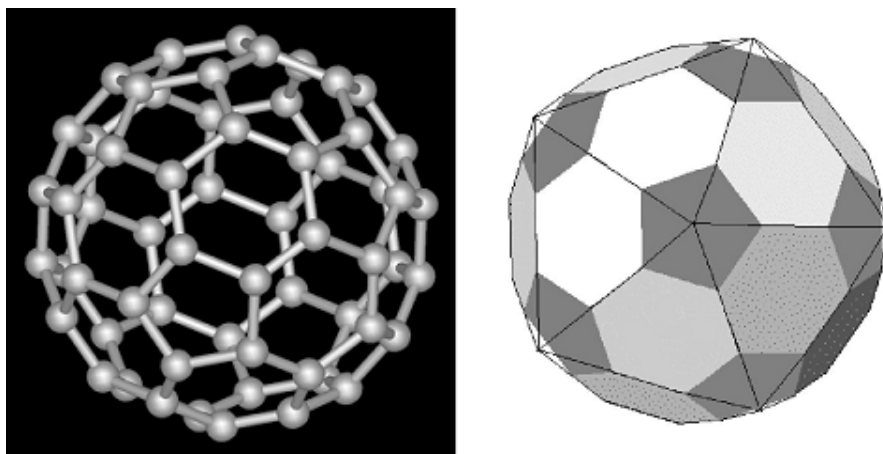


Figure 12: (on the left) **The C₆₀ molecule of fullerene, discovered in 1985.** Its discovery awarded the 1996 Nobel Prize in Chemistry to Smalley, Kroto and Curl. It has a geometry of 20 hexagonal and 12 pentagonal faces, known as truncated icosahedron. (on the right) **The football** has the same geometry: the icosahedron's 12 vertices are cut, transforming into 12 pentagonal faces; the icosahedron's 20 triangular faces become 20 hexagonal faces.



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