

Chemical Analysis as Dematerialization

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Abstract: Chemical analysis is envisaged as an exemplar of laboratory work. Matter, held at a distance within the probe of instruments, is converted there into electronic signals. Matter serves only as prime material for information production. Chemical analysis converts instrumentalized readings into informational statements.

Major chemical thinkers (Auguste Laurent, Justus von Liebig, Jean-Baptiste Dumas, and others) made this conceptual revolution. In mid-nineteenth century, they built a daring theory of radicals. Since that time, molecular chemistry became a combinatorial art and science of radicals. These, groups of atoms with only at first fictional existence, are analogous to phonemes in speech production.

Keywords: *chemical analysis, radical, formula, spectroscopy, synthesis.*

1. Matter for chemistry

I wish to consider in this paper the relationship that chemists entertain nowadays with matter. I shall focus on its manifestations within the sub-discipline of chemical analysis, one of the goals of which is to make a formula correspond to a substance, whether unknown or to be identified. I shall first summarize laboratory practice: it will lead us to partial conclusions. I will present then a parallel with the study of language, which will lead us to a complementary set of conclusions.

Chemistry is routinely defined as the science of the transformations of matter. Does it mean that this science elects for consideration such or such a state, that it deals in particular with the various molecules that have been isolated or synthesized? In doing so, it would risk spreading itself too thinly. There have already been more than 18 million molecules collected in *Chemical Abstracts*. A regrouping into a much smaller number of classes is obviously necessary. In organic chemistry, for instance, such families can be organized with the help of *functions* (such as alcohols, acids, ethers, amides, etc.).

If chemistry then is not so much a science of the too diverse garments of matter, should it be considered instead as the study of their interconversions, *i.e.* of the reactions that atomic assemblies undergo from a given geometric configuration to another one? Not unlike the two sides of a coin, the two aspects do coexist. Chemical *statics* and chemical *dynamics* are these two complementary sides. Chemical science needs both. As we shall see, they share shoving aside the material basis of chemistry. This is their methodological demand. Such a move serves also as a generative *aporia*.

Let us consider the very first stage of chemical work, when it tackles a material sample in order to determine and to state its contents. The set of operations by which the number of compounds present in a sample and their identity are to be determined is termed ‘chemical analysis’.

Let us give a concrete example. For this purpose, I turn to a newspaper article (Folléa 1997, p. 18). It is entitled “30, 000 contaminated teats withdrawn from sale” with the sub-title “A test in ‘Que Choisir’ has established the presence of carcinogenic agents”. The body of the article has this sentence “their dosage draws upon highly sophisticated techniques of chemical measurement termed gas phase chromatography”.

Contrary to the journalist’s rhetoric, gas phase chromatography is a conceptually simple technique, as we shall see. Let us rather consider gas-phase chromatography as a prototypic example of analytical methods in the laboratory, today. We shall present it for its mission, namely to transform chemical matter into information. Thus, I shall try to make explicit what the journalist had found too elaborate for her own understanding (or for that of the readership of *Le Monde*?).

At the beginning, we have on hand teats for baby milk bottles, made of an elastic, plastic and smooth material, of a given color. In order to analyze this material, that presents itself as a solid sample, the very first gesture of the chemist is to transform it into a chemical sample: he needs to disperse, to separate from one another the corpuscles making up the bottle cap. For this purpose, the chemist dissolves a tiny fragment – less than a milligram will be more than enough – in a solvent, a liquid such as alcohol, ether or acetone (yes, the same kind as used to dissolve away nail polish). The ensuing solution contains henceforth, under the aspect of a seemingly homogeneous liquid, all the molecules that were present in the tiny sliver originally removed from the rubber teat. The conglomerate nature of the initial entities, as they existed in the material world of the teat, is already erased by this dissolving act.

The operator then injects with a syringe a fraction of this solution into an oven, in which the mix vaporizes. All the molecules, the solvent molecules and the dissolved molecules originally from the teat, are then carried along by a stream of an inert gas such as helium into a racecourse, strewn with ob-

stacles. Molecules have to go through a long tube, whose length is of the order of a hundred feet, and that has been packed with grains of a polymeric resin, that slows down the gaseous flow. All the molecules that had been injected are borne on this gas flow and, in like manner as debris floating downstream in a torrent, they stick for a short or a long time to local obstacles, just as a tree log is more likely than a twig to be held up by a rock in the whitewater. Another analogy is that of a marathon in which runners would be confronted with obstacles, big and small, here a garbage can to skirt, there a boulder or a wall to climb, and so on.

At the end of such a course, molecules have been sorted out by their size and polarity. Some have gone through faster. Others have been held up for a longer time. In short, a detector at the exit of the chromatographic tube records only, if separation was indeed efficient, homogeneous sub-populations: first the group of the fastest A molecules shows up; it is followed by less rapid B molecules; and so on, and so forth, till the slowest X, Y or Z molecules show up in turn.

That is the manner in which nitrosamines, most often as not quite toxic molecules, carcinogenic on laboratory animals, were shown to be present in the teats of baby milk bottles of the Rémond brand. It caused consternation and a degree of public worry: in the days following the first news, the manufacturer made an announcement answering the charges from the consumer organization (the "Que Choisir" people), the Secretary of State in charge of consumer items ordered some controls to be made, a ban was considered, etc.

But let us return to this workhorse technique of analytical chemistry, gas phase chromatography. It effected a separation amongst the molecules injected into the system, those from the solvent and those from the teat sample: it split an heterogeneous population into homogeneous groups, whose members were all identical in each of the resulting sub-sets.

The separation stage was followed by a detection stage: in one way or another, and let's not worry here about the make-up of the technical device used, the arrival of each pack or group of molecules at the end of their chromatographic marathon triggers an electric signal in a measuring apparatus. A material sample thus gets converted into information, in the form of a peak whose shape contains data, both about the number of molecules involved and about their type.

This is a process of *translation* and it is fundamental. Modern chemistry handles information as much as it handles material change. True, the latter constitutes the subject matter (a deliberate word-play). Nevertheless, as in the real-life case of the adulterated teats, chemists process almost from the outset a piece of information and work on various signals. These electrical ghosts stand for the real material samples. In the example at hand, chromatography, the chemist counts peaks on a screen or on a piece of recording

paper (or has the computer make such a count), providing him with the number of different molecular species that coexisted in the original sample.

The next stage is to identify the compounds present. For this purpose, one resorts to a data bank or, alternatively, a technician injects known samples into the gas chromatograph, under identical conditions: when their peak superimposes with that of an unknown, an identification has been achieved. Even though this is no longer how one actually proceeds, let us remember the principle.

And how does one actually proceed, nowadays? Each of the peaks is analyzed, one after the other. The attendant molecules are hit with a high-energy electron beam that breaks them and ionizes them into fragments. Those atomic assemblies thus bear a positive electrical charge, and a mass spectrometer weighs them according to their mass/charge ratio. Furthermore, the accuracy in the determination of their mass is such that one can determine the elemental composition of each of those ions from the known isotopic abundance for each of the elements (isotopes, let us remind the reader, are atoms sharing the same number of nuclear protons but differing in their numbers of nuclear neutrons). The principle remains the same as previously: attribution of an identity to a chemical species, a fragment from a molecule in the present case, from a 'signature' that unambiguously characterizes it.

Knowing that the molecular unknown, whose overall mass and thus elemental composition are already determined, includes a number of identified fragments, it is now possible to infer how these various component fragments are put together, just as in working out a cardboard puzzle.

Mass spectrometry is a major resource in spectroscopic analysis. Another is nuclear magnetic resonance: absorption of electromagnetic waves, in the range of frequency modulation radio stations, by the magnetic moments of atomic nuclei, when the sample is immersed in a very strong magnetic field, provides a set of absorption peaks, termed a 'spectrum'. Each of the spectral peaks is a signature for a group of atoms that characterizes it usually unambiguously, such as a C=O carbonyl group, a CH₃ methyl group, or a C₆H₅ phenyl group ...

2. The system of signs

In doing so, the chemist has transformed – and I need to emphasize once again that the exact nature of the material devices ensuring such a transduction are of no import for this argument – the material system borrowed from nature into a set of signs and of representations, fit for both computation and sorting out by the brain. He may have resorted to, in complementary or in-

dependent manner to the methodology just described, combining chromatographic analysis with spectroscopic identification by mass spectrometry and nuclear magnetic resonance, determining the structure of an unknown molecule using X-ray diffraction on a crystal, provided that a crystal was available.

In any case, the result consists of a formula and of a three-dimensional model, in which atoms are set according to their microscopic disposition. Their distances are represented on a proper scale. A glimpse shows atoms that stand as nearest neighbors, most of which are linked by chemical bonds. Just like a tax assessor considers a map of a piece of real estate established by a surveyor, or just as an architect looks at his (or her) construction to be on a dummy model, the chemist is able to examine on a molecular model in 'real' space the relations between atoms in a molecule, an entity otherwise so incredibly small that it escapes viewing, even to an instrument-aided eye.

The signalization inherent in the formula or in the model is to a large extent conventional, and it is for the time being the end result of an historical process, which had to a large extent already been completed by the beginning of the twentieth century. The main stages of this development can be identified as: the nomenclature put forward in the 1780s by Fourcroy, Guyton de Morveau and Lavoisier; atomic theory as introduced by John Dalton circa 1810; the notion, anti-positivistic but so masterfully productive, of *radicals* that we owe to Justus von Liebig, August Laurent and Jean-Baptiste Dumas around 1850;¹ and structural chemistry, started in the last third of the nineteenth century by August Kekulé, Archibald Couper, Jacobus Henricus van't Hoff, Achille Le Bel, Louis Pasteur and a few others.

Now to the components of this system of signs: these are the atoms from Dimitri Mendeleev's periodic table, together with the arbitrary typographical symbols that stand for them (C for carbon or Na for sodium) and together with, for each atom, the spatial configuration of the virtual bonds irradiating from it, and ready to link up with other atoms. For instance, there are three classes of carbon atoms, digonal, trigonal and tetrahedral, with two coaxial bonds, three coplanar bonds and four bonds directed to the corners of a tetrahedron, respectively. Thus described, these are idealized concepts, not unlike Platonic archetypes.

These elementary modules are then assembled together into molecules, according to a connectivity, provided by spectral analysis. For instance, the molecule of alcohol (= ethanol) consists of a methyl group (or radical) CH_3 , linked to a methylene radical CH_2 , that is linked in turn to an hydroxy OH radical.

Let us remark, at this stage in our description, that chemical analysis has replaced those immediate phenomenological perceptions, an aspect, a color, a grain or texture, a smoothness or a shine in the light, of a material sample (a

teat, say), by discrete microscopic beings, idealized, postulated, incapable of autonomous existence and perhaps also forbidden any real existence, of a tetrahedral carbon or oxygen atom.

Let us also note the resemblance to features of language. The person I am talking with emits sound waves, whose amplitude and frequency vary over a fraction of a second. Nevertheless, I hear her say one of the phonemes from the English language, for instance that corresponding to the vowel in 'cut' which my ear has easily distinguished from the similar vowel in 'cat'. My brain has spontaneously performed a Fourier analysis, it has used a power spectrum that led me to identify the 'u' of 'cut'. This is a fertile analogy. One can push it quite far, radicals in molecules have an epistemological status resembling that of phonemes in speech utterances.

3. The language of spectroscopy

Let us work over this analogy a little more in depth. In order to identify nitrosamines in the teats of milk bottles for babies, first gas chromatography served to separate them from other molecules in the sample. In a subsequent stage, spectral analysis characterized those nitrosamines, providing a formula for each, together with the relative amounts.

Thus, spectral analysis acts like a language: it associates some signified, the formulas of the nitrosamines in this case, to the signifiers embodied by their spectra. Note that the true basic signifiers and signified are here, on one hand, the discrete absorption frequencies present in a spectrum, and, on the other hand, the groups of atoms, the radicals, present in a molecule.

Let me hasten to point out the difference to a natural language: In spectral analysis we are not dealing with an arbitrary coupling between the sign and whatever is being signified. To the contrary, there is an intrinsic basis for such an association, both empirical and necessary: a given peak, at a certain frequency and of a certain shape, in the nmr spectrum of ethanol signifies methyl, not because I want it to be so, but because it is indeed so. The only arbitrary aspect, here, is denomination, *i.e.* use of the term 'methyl' for this CH_3 group of atoms.

It is important to the present argument that spectral analysis – to which I shall give, without necessity for further justification, the role of an allegory for chemical analysis, taken more generally – has replaced matter by a spectrum (or by a set of spectra). It will rest its further logic on those ghosts exclusively. These ghosts have become the only reality. Henceforth, the original material, or matter, will remain shelved.

At this stage in his work, the chemist holds the spectrum as the only reality. The spectrum stands as the trusted representative of a molecular population, otherwise imperceptible to our sensory organs. The chemist reads the spectrum as an ordered set of signs, that points to a given type of molecule or macromolecule from the material sample.

However, the spectrum, rather than an end in itself, is a mere stage in a process. As soon as it has been read and understood, a molecular object is unveiled behind or underneath it; and in turn it pushes away the spectrum. And this molecular object assumes the shape of one or another representation – in itself arbitrary: one can represent ethanol in dozens of different ways, as a set of touching spheres, or as interpenetrating balls, or yet again as sticks and balls –, which in itself serves as the form that a protean reality temporarily assumes for the chemist. The various models of molecules in the chemical imagination constitute languages akin to the other languages that humans resort to. Chemists agree as to their lexicon and to their construction or syntax, and they are well aware of their conventional nature.

4. Mutation of the laboratory: from work on matter to transformations on signs

Thus the laboratory finishes being the locus for a symbolical work on matter. True, chemists continue performing actual material operations on substances. Besides the most important, their synthesis, they also do their isolation, purification, or yet various modifications aiming at improving, say crystallization, or, in another sphere, that of biological activity, the ability to serve as an efficient drug.

By then, the dematerialized work, if it does not subsume yet the material work, this intellectualized part of the chemists' task has already equal status. Its main tool is at present the computer: to help representing molecular objects by three-dimensional models; to predict vibrational frequencies in the infrared; to predict in like manner the aspects of nuclear magnetic resonance spectra (^1H and ^{13}C , foremost); to map out the electronic density or the electrostatic field at various points in space, relative to the positions of the nuclei in a molecule; to likewise guess the wavelengths of the absorption maxima of visible light and thus predict the color of a molecule; and so on, and so forth.

Going from the macroscopic scale, that of the sensory, to the microscopic scale, that of the postulated molecular object, via the intervening molecular assemblies, is accompanied with another mutation, from experimental observation to theoretical calculations. The goal of chemical analysis, nowadays,

might be defined as the alphanumeric listing of the components in a mixture, in any mixture.

For this purpose, the perspective on matter has become demographic. Any sample is considered as a set, with various sub-sets or sub-populations, comprising a number of molecular individuals. These are determined at an astounding level of precision and accuracy.

The history of chemical analysis, that of the discovery (by Bunsen and Kirchhoff) and of the rise of spectroscopy, can be read thus both as a history of the progressive rise in sensitivity of measurement and as a history of the gradual distancing from reality: it has jettisoned the immediate properties in favor of the mediated properties.

When in the eighteenth century Gabriel Venel wrote the *chemistry* entry for the *Encyclopédie*, two kinds of analysis were being performed, analysis by fire, and analysis by menstrues (*i.e.* by what we now term 'solvents'). These two analytical modes have given rise to spectral analysis, and to chromatographic analysis, respectively; but at a cost, that of a removal.

Take the case of chromatography: in between the chromatogram and the material sample that it represents, at first stands a solvent; then, a black box filled with grains made of various resins, the 'support'; followed by another solvent or eluent, whose role is to sweep the molecules adsorbed on the chromatographic support; then one finds a detecting device (measuring, for instance, changes in the refractive index); a converter producing an electrical current, leading into another black box, packed with electronic instrumentation and digitizers: signal amplifiers, adding machines, data-smoothing and -integrating devices and software, etc.

To give a full picture, as a rule samples have become minuscule, in amounts generally between micrograms and milligrams. One may safely conclude that present-day chemists 'handle' mostly mental representations. The chemical laboratory, more than the site of transformations of matter, has become predominantly a production center for concepts.

5. Should chemical synthesis be held as a rematerialization?

It is customary to pit analysis and synthesis as the two sides of a coin, as activities complementary to one another and to some extent symmetrical. The former clearly enjoys historical priority. The latter can be dated, referring only to milestones, to Wöhler's synthesis of urea in 1828, with the subsequent anti-vitalism slant that was given to it, and to the syntheses by

Berthelot of prototypic molecules such as acetylene and benzene during the second half of the nineteenth century.

The above description of analysis as a process of dematerialization might lead the reader to expect, as a contrast and by way of a satisfactory and expected resolution at the end of this paper, a presentation of synthesis as the indispensable rematerialization; which, of course, is true to some extent, but only in a rather naive and superficial approach. Each of the steps in the multi-stage synthesis of a complex natural product, such as those of quinine, strychnine or taxol, translates into access to an intermediate that can be weighed and identified through its spectroscopic analytical data, in the manner of a newborn.

However, the reality of the synthetic effort is elsewhere. It is an algorithmic process, it is a logical concatenation (computer-assisted too) in which radicals are gradually added to a structure, to that particular molecular architecture being erected. In synthesis, just as in analysis, idealities are dominant and they rule over any materiality. Matter dares to show up only at the very end, when the overall yield (or that for an individual step) is determined.

The reader may protest: is there no return to reality, to this proto-form matter, sometimes lumpy, sometimes fluid, that can take up so many incredibly diverse and unpredictable aspects, and which is to be found contained by and in the glassware that chemists handle in their laboratories?

The answer not only is "yes", it is also an interesting one! The molecular object, this representative of the molecule in the form of variously colored balls (atoms) connected by sticks (bonds), this molecular model that the chemist holds in his hands, or that he examines on the screen of his computer terminal, has the function for today's chemists of a kind of *substitutional hardware*. The molecular object is thus a close parent to the transitional object, as defined by psychoanalysts such as D.W. Winnicott.

Another easy and obvious temptation should be mentioned: to seek a rematerialization in chemical industry, since chemical science in academic laboratory seems to have jettisoned the materiality of chemistry. This ploy won't work though! In spite of chemical industry harboring some of the high temples of empiricism, any visitor of a chemical plant becomes quickly aware that the only matter he will see is either some of the primary material or some of the finished and packed product. The rest remains invisible, it is the province of chemical engineers who stand close guard over transfers of heat and material through large pipes.

The reactors proper, the interconnecting ducts with the occasional outlet of water vapor fumes, are all controlled from a set of terminals and gauges for pressures, temperatures, viscosities, etc. at various locations in the huge network: matter has been screened off from the viewer by a complex hydrography, monitored and directed via computers.

Thus, we are led to the conclusion that chemistry is a science of matter in a formal sense only. It is, to a much greater extent, a science of mind. Like music, chemistry is a combinatorial art and science. In the same way as music goes beyond acoustics, chemistry transcends matter and has the intellect as its dwelling place.

Note

- ¹ It is considerably more fruitful to think of, say the ethanol molecule C_2H_6O as the union between the two radicals, between the two fictitious species, ethyl C_2H_5 , and hydroxy, OH , than to conceive of it as the adduct (which it is!) of the two very real and existing molecules ethylene C_2H_4 and water H_2O .

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Acknowledgment

I am pleased to express my gratitude to Ms. Françoise Monnoyeur for permission to hereby translate and adapt a chapter, originally in French, of a forthcoming collective monograph on Matter.

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