FEATURE ARTICLES

An "Analysis" of Analytical Chemistry

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Received July 15, 1986

Current definitions and usages of the expressions chemical analysis and analytical chemistry are compared. Robert Boyle's definition of chemical analysis, the determination of the composition of substances, is considered adequate. Analytical chemistry may be considered as a branch of applied chemistry comprising the inorganic and/or organic chemical processes and/or physical operations used in making chemical analyses. Included is information on the number and nature of abstracts for analytical chemistry appearing in Volumes 103 and 104 of *Chemical Abstracts*. Possible improvement is suggested for the cross-references to nonanalytical abstracts.

Chemical Abstracts, the key to the world's chemical literature, reports biweekly the new information in chemistry and chemical engineering. For the convenience of users, the abstracts are classified and issued in 80 named sections.

Does this segregation of information represent 80 kinds of chemistry? Only 20 of the 80 section headings contain the word chemistry (in 1986). In 10 of these cases chemistry is a separate word, but in the others there are prefixes, such as bio-, electro-, immuno-, photo-, and thermo-.

Usually the basic chemistry of carbon and all of its compounds (with a few exceptions, such as limestone) is considered organic chemistry and that of all of the other elements of the periodic table and their compounds as inorganic chemistry. The great archival depositories of this information are the respective treatises of Beilstein and Gmelin. Where, then, does this leave analytical chemistry and the other sections having the separate word chemistry as part of their titles?

The expression analytical chemistry has been, and still is, widely used in chemical publications. The best-known examples are the word titles of periodicals, technical reports, reference works, and textbooks. Perhaps the most noteworthy of such uses are the titles of the last 2 of the 80 sections of *Chemical Abstracts*, namely, 79, Inorganic Analytical Chemistry, and 80, Organic Analytical Chemistry.

In this presentation the word "analysis" is used in the general sense of resolution into constituent parts rather than in the usual chemical sense. The objective is to examine the status in the chemical literature of the expression analytical chemistry. At least the following questions arise: What is its definition? Is it a kind of chemistry other than inorganic and organic? Can one differentiate between analytical chemistry and chemical analysis?

The intention, then, is to consider present practice with respect to analytical chemistry, chemical analysis, and the nature of the contents of the analytical abstracts in *Chemical Abstracts*.

The comments and suggestions presented are based on two extensive associations with the chemical literature. The first has involved over 50 years with the general chemical literature, as outlined in the five editions of the book *Chemical Publications*.[21] The second has involved 25 years as editor/advisor for Sections 79 and 80 of *Chemical Abstracts*, that is, with what is contained therein as analytical chemistry. The kinds of publications include primary sources (periodicals, technical reports, and patents), and secondary sources (periodicals, treatises, monographs, and textbooks).

CHEMICAL ANALYSIS

According to Moore,[28] Robert Boyle (1627-1691) was the first to use the expression chemical analysis in its modern sense. By this Boyle meant the determination of the composition of substances, a definition that seems difficult to improve. It implies nothing, of course, of how or by what means a determination is accomplished. Determination of *what* is in a substance is qualitative analysis, and *how much* of one or more components is quantitative analysis.

Many decades later Ostwald[31] came close to Boyle's definition in the statement "It is the *art* of recognizing different substances and determining their constituents." A recent statement[3] almost repeats Boyle's definition: "the determination of the qualitative and/or quantitative composition of substances and materials".

More wordy is the definition of Kaiser:[11] "Chemical analyses are information processes planned...with the aim of obtaining knowledge about the composition of substances under investigation."

The expression chemical analysis has been widely used in the titles of textbooks. Unless the title cannot be misunderstood, it should include the word chemical, as *Qualitative Chemical Analysis* and *Quantitative Chemical Analysis*. Several books, having nothing to do with chemistry, have appeared with the title *Quantitative Analysis*. Likewise, a book titled *Instrumental Analysis*[35] might better be *Instrumental Chemical Analysis*.

Three texts, clearly analytical in content, are titled *Exercises in Quantitative Chemistry*,[29] *Introduction to Quantitative Chemistry*,[12] and *Introductory Quantitative Chemistry*.[30] Could not these titles imply that only analytical processes and operations are quantitative in nature?

As long as writers use the expression chemical analysis in the sense defined by Boyle, there is no question of clarity or

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brevity. An early example was the book by Lampadius.[15] Trouble begins in trying to specify kinds of methods, areas involved, and chemistry utilized. The 25 analytical terms cited previously[25] are examples justifying the question, What mean these words? Are they clear? What property is measured? What kind of chemistry was used to render measurement feasible. Were separations necessary? If so, what kind?

In order to emphasize the distinction between the chemistry and the physics of methods of quantitative chemical analysis, I have adopted the following outline for the two editions of my textbook.[23]

SAMPLE

Selection and Preparation. To make a chemical analysis one needs access to the material to be analyzed. It may serve as is, that is, in situ or in vitro, as in checking the pH of a fish aquarium or in making a spectrometric surface analysis. In contrast, often a bulk sample is obtained, as in sampling the mountains of Utah for potassium or a car of 50 tons of coal for its heating value. Preparative details are involved for obtaining a 1-g portion to be used in the actual determination.

In many cases certain preliminary transformations are necessary, such as fusion, dissolution, pH adjustment, oxidation, reduction, complexation, and other reactions. These are chemical processes.

DESIRED CONSTITUENT(S)

Separation. Unless one can measure directly the desired constituent, or something chemically equivalent to it, some separation is necessary,[24] such as absorption, adsorption, centrifugation, dissolution, distillation, electrodeposition, evaporation, precipitation, and others, particularly chromatography. Again, these are chemical (except the mechanical centrifugation).

Measurement. In quantitative work, measurement, or the determination of a physical property, is the final operation step. Common properties are mass, volume, pressure, and a variety of electrical, optical, and other properties (see ref 23b, p 167). Measurement may be considered as the determination of the number of times the unit of measurement goes into the unknown or the assignment of a number to the physical property measured. No chemistry is involved, for the operation is physics. As one measures with an instrument, all measurement is instrumental.

It may be noted that the chemical processes, unless carefully controlled, are potential sources of error in an analysis. In contrast, if the meter is calibrated and properly adjusted, making reliable readings should not be difficult. Generally, separations are to be avoided, although a new book[35] states, "All analyses require separations."

Lundell's paper,[16] "The Chemical Analysis of Things as They Are", is a memorable overview of the importance of understanding and utilizing the chemistry involved in analyzing multicomponent systems. Later, he and Hoffman[17] amplified these ideas in the book *Outlines of Methods of Chemical Analysis*. It is a concise unique organization of chemical information applicable in developing methods of analysis for specific situations. As stated in the preface, "An attempt has been made to feature *chemical analysis* rather than chemical *determinations*." In both publications the term determination is limited essentially to the operation of measurement. Today usually a method describing a procedure for the determination of iron in an ore, for example, includes any necessary chemical processes made preliminary to measurement.

Walton's text[43] seems unique in stating "This book is about the chemistry in analytical chemistry...(that is) chemical reactions and chemical separations." Methods of measurement are not included. The subjects selected to illustrate this chemistry include (a) separations (by precipitation, evaporation, solvent extraction, and ion exchange) and (b) titrations (by neutralization, oxidation–reduction, precipitation, and complexation). Included are the reactions of indicator compounds.

Although Walton was the first to emphasize chemistry this way in a textbook, various earlier works stressed the same general view in detailed and extensive discussions of the chemistry in methods of chemical analysis. Examples of such well-known texts are those of Willard and Diehl,[46] Treadwell and Hall,[42] and Washington.[45] Two monographs covering similar chemistry are those of Hillebrand and Lundell[8] and Mellor and Thompson.[26]

I have discussed the chemistry involved in one area, colorimetry.[22] A simple example of applying chemistry is the spectrophotometric determination of fluorine in organic compounds by means of heteropoly reactions.[4] In general, analysts use the inorganic and/or organic chemistry needed to render desired constituents detectable, identifiable, and/or determinable.

As a part of their analytical maturation and as a reminder that there is chemistry in this instrumental age, an analysis of a tombstone-grade granite rock, by the methods of Washington,[45] should provide graduate students some appreciation of the following items: (1) the significance of the chemistry involved in the premeasurement stages of the analysis; (2) the care required in all of the operative details in order to achieve what Washington considered a satisfactory analysis, that is, a total of 100.00 ± 0.25% for some 20 constituents; and (3) some knowledge of the general nature of the material that may well mark the final resting place of their nonvolatile remains (the "dust" of Genesis 3:19).

In another text Walton and Reyes[44] state "This is a textbook of instrumental analysis." Yet 4 of the 12 chapters deal with chromatography, which (the authors state) "is a name given to a family of methods for separating complex mixtures". These chapters would seem, therefore, to belong in the chemistry text.

It seems reasonable now to conclude that quantitative chemical analysis always involves measurement (physics) and much of the time some inorganic and/or organic chemistry. An alliterative "6 M" summary might be "The *M*eans and *M*ethods of *M*aking *M*eaningful *M*easurements on *M*aterials".

ANALYTICAL CHEMISTRY

In *A History of Chemistry from Earliest Times* Brown,[2] following consideration of a prehistoric period, discussed the following periods: Alchemical (1500 B.C. through 1650 A.D.), Iatrochemical (1500–1700), and Phlogiston (1650–1775). This coverage of more than 30 centuries mentions discovery and use of a great stock of chemical information. Included are many items of analytical interest, as cited by Laitinen and Ewing.[14] Szabadvary[39] states that chemical analysis, in simple fashion, was practiced for 2000 years before Bergman (1735–1784), but it was he who gave it the status of a separate branch of science—analytical chemistry. Although this expression came into more or less general use, few writers committed themselves to a definition.

Szabadvary and Robinson[40] state "In the works of Bergman we find the earliest form of textbook, in that they give a methodical summary of the processes of analytical chemistry grouped according to the nature of the substances analyzed." The same authors state that Pfaff's book[32] was "The first really general and comprehensive textbook". Wöhler's book is material oriented.[48]

Many of the early processes, presumably needing some analytical testing and control, included amalgamations, calcinations, combustions, crystallizations, cupellations, digestions,

dissolutions, distillations, evaporations, percolations, refinings, roastings, smeltings, sublimations, and probably others.

To Lavoisier (1743–1794) may be given credit for laying the theoretical foundations for the current quantitative period of chemical history (1775+). His work, along with that of many others, cleared the air of phlogistonism and set the direction for developing our present knowledge of the chemistry of the elements and their compounds.

A statement by Ellis[5] seems to equate chemical analysis and analytical chemistry: "The specific purpose of analytical chemistry is the resolution of a compound or mixture into its constituent parts or elements, which are qualitative when the nature only of the constituents is determined, or quantitative when their actual quantity or proportion is ascertained."

The statements of Ostwald and of Ellis cover modern qualitative and quantitative chemical analysis. Neither one suggests that analytical chemistry is a kind of chemistry other than inorganic or organic.

Several other efforts at defining the area are of interest. Walton[43] states that "essentially analytical chemistry is an applied field". This view corresponds to a dictionary definition: "Analytical chemistry is a kind of applied chemistry."

More detailed is Considine's statement:[3] "Analytical chemistry is that branch of chemistry which is concerned with the detection and identification of the atoms, ions, or radicals of which a substance is composed, the compounds which they form, and the proportion of these compounds which are present in a given substance."

Meites and Thomas[20] state "Analytical chemistry is that branch of chemical research which has the development and improvement of practical analytical procedures as its goal." Hume[9] thinks that it is a point of view, an intellectual attitude, a way of attacking problems, a discipline in its own right.

More questionable is Bard's recent statement:[1] "Analytical chemistry is the science of the measurement and characterization of systems." This does not isolate analytical chemistry. For example, a number of ASTM methods involve measurements, such as tensile strength, hardness, and tristimulus color values, to be used in characterizing the systems measured. These methods are not chemical analysis. Furthermore, one does not measure anything in using the Fresenius system of qualitative analysis for ions. Questionable, too, is the remark "To develop an analytical technique we need physics and computer science." Again, the Fresenius procedures need little, if any, physics, and the author thought that his students had devised new spectrophotometric methods without resort to computers.

As a different definition of analytical chemistry, Massart and Hopke[18] suggested recently, "The chemical discipline that uses statistical and other methods employing formal logic (a) to design or select optimal measurement procedures and experiments, and (b) to provide maximum chemical information by analyzing chemical data".

Ewing[6] states "Analytical chemistry may be defined as the science and art of determining the composition of materials in terms of the elements or compounds contained in them." This is essentially a combination of the definitions of chemical analysis by Boyle and Ostwald.

The first use of the expression analytical chemistry in a journal title was by Fresenius for *Zeitschrift für Analytische Chemie* in 1862. The *Journal of Analytical Chemistry* was started in 1887, with a change of title in 1891 to *Journal of Analytical and Applied Chemistry*. The best-known example today is *Analytical Chemistry*. From 1929 to 1947 it was *Industrial and Engineering Chemistry, Analytical Edition.*

The latest analytical journal (1985) is *Analytical Sciences.* This title implies extending the usual analytical coverage to "Quantitation with respect to oxidation state, crystalline form, reaction rates, and the like". One wonders if nonanalytical science is contemplated.

Table I. Data on the Abstracts and Cross-References in Sections 79 and 80 for Volumes 103 and 104 of *Chemical Abstracts*

section	abstracts			cross-reference
	general	books	patents	
	Volume 103			
79	2241	35	330	1559
80	586	3	70	1041
total	2827	38	400	2600
	Volume 104			
79	2637	55	546	1717
80	920	10	151	1024
total	3557	65	697	2741
grand total	6384	103	1097	5341

General abstracting journals have long used analytical chemistry as a subdivision. Thus, by 1863 *Chemisches Zentralblatt* had a section, Analytische Chemie. In *Chemical Abstracts* Section 7 was Analytical Chemistry from 1907 through 1961. Beginning in 1962 it became Section 2 (to emphasize the importance of analytical information in subsequent sections?). With the adoption of 80 sections in 1967, the general analytical material was divided, Section 79 becoming Inorganic Analytical Chemistry and Section 80 becoming Organic Analytical Chemistry. Many items on applied analysis in specific areas are cited in cross-references to other sections (see later).

Many textbooks have had, and still have, analytical chemistry as part of their titles. An early and popular example was Treadwell's *Kürzes Lehrbuch der Analytische Chemie.*[41] It became well-known through translations by Hall of at least nine editions, with the title *Analytical Chemistry.* The subtitle for Vol. I was *Qualitative Analysis*, and for Vol. II, *Quantitative Analysis.*[42] A number of current American texts, such as that of Skoog and West,[36] carry the title *Analytical Chemistry* or some variation, such as *Fundamentals of ..., Introduction to ...*, and *Advanced ....* Four of the five comprehensive treatises include analytical chemistry as part of their titles.[7,13,33,37,47] Do all such titles indicate coverage of qualitative and/or quantitative material? This uncertainty is not inherent in the title of Rüdisüle's treatise.[34] Combined treatment is illustrated in Swift's text.[38]

In Meites's *Handbook of Analytical Chemistry*,[19] handbook is not used in the sense of the Fresenius and Jander Handbuch. Rather the work is a compilation of numerical data and a variety of condensed information thought to be of interest to analytical chemists.

Ihde's statement[10] comes close to equating analytical chemistry and chemical analysis: "It is not incorrect to ascribe to analytical chemistry a position of primary importance, since only through chemical analysis can matter in its variety of forms be dealt with intelligently." In a similar vein, von Meyer,[27] in discussing the history of various divisions of chemistry, took up analytical chemistry first because, he stated, "Analyses support nearly all chemical research and development."

Might one now conclude that analytical chemistry comprises all of the inorganic and/or organic chemical processes and/or the physical operations used in making chemical analyses? Perhaps an orismologist is needed here.

CONTENT OF ABSTRACTS FOR ANALYTICAL CHEMISTRY

Since 1966 *Chemical Abstracts* has listed separately in Sections 79 and 80 the abstracts of (a) general articles, technical reports, conference proceedings, and dissertations;

Table II. Distribution, by Section Numbers, of the Cross-References among the 80 Sections[a] of Volume 104 of *Chemical Abstracts*

number of references			
0	1–5	6–10	>10
	Section 79		
3, 5, 6, 7, 8, 10, 11, 12, 13, 14, 15, 16, 18, 21, 23, 24, 26, 27, 29, 31, 32, 33, 34, 44, 62	1, 2, 4, 22, 25, 28, 30, 35, 36, 37, 38, 39, 41, 42, 45, 49, 50, 54, 63, 64, 65, 70, 74, 77	40, 46, 48, 52, 67, 69	19, 20, 43, 47, 51, 53, 55, 56, 57, 58, 59, 60, 61, 66, 68, 71, 72, 73, 75, 76, 78
	Section 80		
3, 6, 7, 8, 10, 12, 13, 14, 15, 16, 18, 24, 27, 30, 32, 53, 54, 56, 65, 70	1, 2, 4, 11, 21, 23, 25, 26, 28, 29, 31, 33, 38, 39, 47, 49, 50, 52, 55, 57, 58, 62, 63, 67, 68, 71, 74, 75, 76, 77, 78	22, 40, 48, 60	5, 19, 20, 34, 35, 36, 37, 41, 42, 43, 44, 45, 46, 51, 59, 61, 66, 69, 72, 73

[a] Missing numbers (9, 17, 64, 79, 80) are for sectional cross-references.

(b) announcements of new books; and (c) patents. Under (a) the general order is reviews, apparatus (instruments), reagents, separations, and methods for the detection or determination of constituents in or of materials. There is no classification in terms of kinds of information in each abstract.

Two alternatives serve instead of specific classification. The first is the cross-references to nonanalytical sections (discussed later). The three sectional cross-references (9 Biochemical Methods, 17 Food and Feed Chemistry, and 64 Pharmaceutical Analysis) represent a kind of classification, but of these three only Pharmaceutical Analysis is entirely analytical.

The second alternative is *CA SELECTS*, the biweekly bulletins that contain the complete abstracts and citations of *Chemical Abstracts* for recent papers, patents, and other publications on particular topics. Some 165 topics are now covered (1986). New ones are added as they are requested and can be supported. A recent analytical addition is Spectrochemical Analysis.

In classification contrast, the British *Analytical Abstracts* classifies its material as follows: (A) General Analytical Chemistry; (B) Inorganic Chemistry; (C) Organic Chemistry; (D) Biochemistry; (E) Pharmaceutical Chemistry; (F) Foods; (G) Agriculture; (H) Environmental Chemistry; and (J) Apparatus, Techniques. Various subdivisions make the abstracts for more specific areas readily available.

In order to try to determine the nature of the material covered in the three parts of each section, the abstracts for Sections 79 and 80 in Vol. 103 and 104 of *Chemical Abstracts* were examined for a basis of classification. The following listings were adopted: entirely physical (instruments); entirely chemical; physical and chemical; and unclear. Sorting the abstracts of (a) into these four categories by computer did not prove feasible. So remains unanswered the question of the relationship of the proportion of entirely physical abstracts to the current emphasis in texts and teaching on instruments and experimental physics.

The titles of books may or may not indicate whether the material is entirely physical, entirely chemical, or a combination of the two. One titled *Analytical Chemistry* may be either qualitative or quantitative in content or, less likely, a combined treatment. To be certain, the table of contents may be consulted. Parts of multivolume treatises usually are clear.

A United States chemical patent listed in *Chemical Abstracts* will be for a machine (mechanical or electrical), a process, or a composition of matter. A new spectrophotometer or balance is an instrument, but is a new apparatus, such as molecular still? Chemical processes and compositions of matter are clearly chemistry. Presumably foreign patents may be similarly classified.

CROSS-REFERENCES IN CHEMICAL ABSTRACTS

In every issue of *Chemical Abstracts* Sections 79 and 80 contain many cross-references to other sections. These cross-references are to publications that are primarily not analytical chemistry, but they do contain items which the abstractors considered of possible analytical interest. The documents cited include papers, reports, and patents. Inclusion of such references depends upon the abstractor's breadth of perception of what might be of analytical significance in modern chemical analysis.

Many of the titles in the references do not themselves indicate what may be of interest. Examples of uninformative titles of cross-references follow: Porous Mullite; Calcium Hydrosilicate; Electronic States in Glassy Metals; New Insights with High Resolution; and Solid State Electrolytes. In such cases one wonders what the abstractor thought might be of interest to analysts. Was it a method of analysis, a special kind of chemical treatment, the method of measurement, or something else? Some kind of tagging to indicate the kind of items would be helpful. The abstracts cited generally provide the relevant information, but they may not.

Two examples of at least partially informative titles are "Spectrographic Determination of Antimony" and "A Colorimetric Procedure for the Determination of Aldehydes in Sea Water".

In Table I the total number of abstracts and cross-references are shown for Sections 79 and 80 of Vol. 103 and 104 of *Chemical Abstracts*. The 26 issues of these two volumes cover one year, that is, the last six months of 1985 and the first six months of 1986.

The data of Table I raise an interesting, if disturbing, question. Out of all this array of new information, what is relevant to what was being taught in a general course on quantitative chemical analysis during the academic year 1985–1986?

As an example of the distribution of cross-references among the 80 sections of Vol. 104 of *Chemical Abstracts*, the section numbers (in groups) are listed in Table II. The sectional cross-references (9 Biochemical Methods; 17 Food and Food Chemistry; and 64 Pharmaceutical Analysis) provide no direct help, although testing and analysis are used extensively in these areas. There are nearly as many cross-references as general abstracts.

In general, the most cross-references are to sections dealing with various areas of applied chemistry, and the least (or none) to theoretical areas. Sections in Vol. 104 having many cross-references are 51 Fossil Fuels, Derivatives, and Related Products (219); 59 Air Pollution and Industrial Hygiene (544); and 61 Water (637). In all three areas testing and analysis are very important. In Section 79 there are no cross-references to 25 of the other sections, and in Section 80 the number is 20.

The distribution of cross-references in Vol. 103 is much the same as that shown in Table II for Vol. 104.

As the section numbers shown in Table II are scattered among all five parts of *Chemical Abstracts*, one would need access to a complete set of the journal to check all of the cross-references.

The comments and suggestions on analytical chemistry may be summarized as follows:

(1) Analytical chemistry is not a distinct kind of chemistry. Any chemistry used to render constituents detectable, identifiable, and/or determinable is inorganic and/or organic.

(2) Boyle's definition of chemical analysis seems adequate after three centuries of use.

(3) Several definitions of analytical chemistry seem imprecise and inadequate. A new one is proposed: that branch of applied chemistry comprising the inorganic and/or organic chemical processes and/or the physical operations used in making chemical analyses.

(4) Current writing seems to equate chemical analysis and analytical chemistry.

(5) Measurement does not involve chemistry. As all measurement is instrumental, the word is not a differentiating term.

(6) By using more precise titles for articles, patents, books, and other publications, authors could contribute to better understanding and, thereby, improve subject indexes and facilitate retrieval of information, both by manual searching of printed indexes and by online searching of chemical databases.

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