# Contents

## Summary outline of the complete BC2 classification

2 Physical forms & forms of arrangement of documents

3 Phenomena: subjects of knowledge

* For documents covering a subject from a multi- or non-disciplinary viewpoint.

4 Prolegomena

* Classes concerned with the organization and communication of knowledge and information and which are preliminary to a general bibliographical classification of all knowledge.

Methods of enquiry... Disciplines in general

Information science & technology... Libraries...

Disciplines, forms of knowledge

A Philosophy & logic

AM Mathematics & statistics

AY Science

B Physical sciences

E Biological sciences

Human sciences & human studies

H Anthropology.. Health & medicine.. Psychology..

J/T Social sciences & humanities

U/V Technology & useful arts

W/Y The Arts

Z Religion

* Alternative to locating at P.

# Second outline of the complete BC2 classification

2 Generalia: physical forms & forms of arrangement of documents

3 Phenomena: objects of knowledge
* For multidisciplinary or non-disciplinary treatments of a topic.

4 Prolegomena to a general classification
* Classes concerned with the organization and communication of knowledge & information.
. Methods of enquiry.. Disciplines in general..
. Information science & technology
. . Primarily reference retrieval.. Computerized services..
. . Primarily document retrieval.. Libraries..

Disciplinary classes: forms of knowledge..

A . Philosophy.. Logic..

AM . Mathematics.. Statistics..

AY . Sciences, natural sciences

B . . Physics

C . . Chemistry

D . . Astronomy & Space sciences

DH . . Earth sciences

. . . Geophysics.. Geology.. Hydrology.. Meteorology..

. . . Geography.. Regional.. Systematic..

E . . Biological sciences

EK . . . Microbiology

F . . Botany

G . . Zoology

GR . . Applied biology

. . . Agriculture.. Animal exploitation..

GY . . Ecology: general & human

. Human sciences & human studies

H . . Anthropology.. Human biology.. Physical anthropology..

HH . . Health & medicine.. Psychology

I . . Psychology & psychiatry

J . . Education

K . . Society

K9Q . . . Perspectives: Sociology.. Social anthropology..

KAH . . . Social ecology & environment.. Demography..

KC . . . Social processes: Change.. Social behaviour..

KK . . . Social structure

KLK . . . . Collectivities: Groups.. Classes.. Family..

KRS . . . . Inclusive societies.. Non-literate.. Literate..

KW . . . Customs.. Folklore & mythology..

LA . . Area studies..

LB . . Human geography * Alternative to DX

LC . . Travel & description.. Topography..

LD . . History

LE . . . Auxiliary studies: Archaeology..

LF . . . Prehistory

LG . . . *Kinds of history by social activity*
* With alternatives for special kinds (eg, Economic)

LJ . . . *By period*

. . . . Ancient.. Modern..

. . . *By ethnic group*

LM . *By territorial group*

M . . Favoured country * Home country of library.

N . . Other countries * By Schedule 2 Place.

O . . Local history (Alternative)

. Biography

P Religion.. Occult..
Morals & ethics

Q Social welfare.. (Special groups) Criminology..

R Politics.. Public administration..

. International relations..

S Law

T Economics.. Business administration & management..

U/V Technology & useful arts

. Equipment.. Plant.. Instrumentation..
. Systems engineering.. Control.. Computers..
. Testing.. Maintenance.. Production technology..
. Materials handling.. Packaging.. Storing..
. Energy technologies
. . Nuclear.. Electrical.. Thermal.. Mechanical..
. Construction technology
. . Civil engineering.. Architecture.. Physical planning..
. Environmental technology.. Safety technology..
. Transport technology.. Land.. Water.. Air.. Space..
. Military science & technology
. Minerals extraction technology.. Oil & gas..
. Process industrial technology.. Chemical technology..
. Manufacture of special products

VS Household arts, house & home & garden..
Corporate housekeeping.. Catering..

VV Recreative arts.. Games.. Sports.. Tourism..

W The Arts.. Visual arts.. Applied arts.. Fine arts..

WM Mixed media arts.. Temporal arts.. Performing arts..

WP Music.. Theatre.. Dance theatre.. Cinema..

WTU Broadcasting arts.. Radio.. Television..

X Philology.. Linguistics.. Literature..

Z Religion.. Occult..
* Alternative to P.

# Volumes in the series

The second edition of the classification will be complete in twenty-three volumes. Fourteen have been published so far and are identified by their dates of publication.

| | |
|---|---|
| | Introduction and Auxiliary schedules. 1977 |
| Class 2/9: | Generalia, Phenomena, Knowledge, Information science and technology |
| Class A/AL: | Philosophy and Logic. 1991 |
| Class AM/AX: | Mathematics, Statistics and Probability. 1993 |
| Class AY/B: | General science and Physics. 1999 |
| Class C: | Chemistry. 2012 |
| Class D: | Astronomy and Earth sciences |
| Class E/GQ: | Biological sciences |
| Class GR/GZ: | Applied biological sciences: Agriculture and Ecology |
| Class H: | Anthropology, Human biology, Health sciences, Medicine. 1980 |
| Class I: | Psychology and Psychiatry. 1978 |
| Class J: | Education. 1990 |
| Class K: | Society (including social science, sociology, social anthropology, customs, folklore and mythology). 1984 |
| Class L/O: | History (including area studies, travel and topography, and biography). |
| Class P: | Religion, the Occult, Morals and ethics. 1977 |
| Class Q: | Social welfare (including criminology). 1994 |
| Class R: | Politics and Public administration. 1996 |
| Class S: | Law. 1996 |
| Class T: | Economics, Management of economic enterprises. 1987 |
| Class U/V: | Technology and Useful arts (including household management and services). |
| Class W: | The Arts. 2007 |
| Class WP: | Music. |
| Class X/Y: | Language and Literature. |

# The Bliss Classification Association

The Bliss Classification Association is an association of users and supporters of the Bibliographic Classification. It promotes the development and use of the classification, publishes official amendments, enables users to keep in touch and exchange experience, and gives them a say in the future of the scheme. It is a non-profit organisation, founded in 1967, with members all over the world.

An Annual General Meeting is held each year in London. The Association holds occasional other meetings, organises training in the use of the classification, raises funds, and publishes the annual *Bliss Classification Bulletin*.

The *Bulletin* carries amendments to BC2, news about the Association and the development of the scheme, articles on classification, and reviews. It is available only to members. Membership is open to all organisations and individuals interested in BC2.

Full details of the Association, with contact information, list of committee members and a membership application form, are on the Association's web site at

www.blissclassification.org.uk

The Association is pleased to hear from users and supporters of the classification and to answer questions about it. There is an electronic discussion list, which can be used by email or viewed on the Web, which anyone interested is encouraged to join. Its home page is at:

https://www.jiscmail.ac.uk/cgi-bin/webadmin?A0=lis-bca

# Introduction to Class C
# Chemistry

## 1 Introduction

**1.1** This schedule is the result of a rigorous and detailed analysis of the vocabulary of chemistry, which uses the techniques of facet analysis. It is a radical revision and expansion of Class C in the first edition of the Bibliographic Classification (BC1) (1). The general reasons for making the revision so radical are given in the Introduction and Auxiliary Schedules to BC2 (2). The particular changes in this class are considered in Section 14 below.

**1.2** The schedule, like that of all the classes of BC2, is designed to perform several major functions:

**1.21** It serves as a practical tool in the management of chemical documentation and information. Initially developed as a library classification scheme, that remains a fundamental purpose of BC2, in which role it supports both browsing and retrieval functions. It makes possible the organization of a comprehensive collection both of documents on chemistry (whether books or other media) in a clear and logical sequence on library shelves, and of entries for them in catalogues, bibliographies and other linear displays. Additionally its logical structure makes the locating of any particular subject within chemistry, however complex, highly predictable, a central requirement of any instrument for information retrieval. The way in which the classification is structured, and the application of the facet analysis methodology to create that logical structure, form the major themes in most sections of this introduction.

**1.22** Search tools with faceted features have recently become more widely adopted, both in conventional library and information work, and in commercial search applications. Many of the discovery tools now used in academic library catalogues exploit the structured nature of bibliographic data and offer faceted browsing and navigation as standard, and faceted search tools in e-commerce are very common. BC2 provides a model for faceted subject tools, and this introduction contains a statement of established principles and methodologies, particularly when dealing with more complex aspects of subject representation.

**1.23** Finally, this schedule acts as a highly structured and detailed map of the concepts in the field of chemistry, and a substantial terminological resource. This may be used as the basis for the construction of thesauri or other aids for searching an information store, through the control of synonyms and the comprehensive display of the connections of all kinds between different concepts. This function is considered further in Section 13.

**1.3** The central feature of a library classification, as distinct from any other kind of knowledge organization system, is that it can present all its concepts, simple or complex, in a single, one-dimensional sequence. Most of the subject classes represented by books, journal articles, research reports, etc. are compounds of several different concepts and could equally well be classified in a number of quite different ways. For example, a work on radiography in the diagnosis of stomach cancer could go equally well under radiography, diagnostic techniques, stomach, or cancer. Such a compound reflects twenty-four different locations in a linear sequence, all of them logically justifiable and sensible (twenty-four is the factorial product of four and represents the different combination orders in which the four concepts could be taken).

**1.4** While catalogues, bibliographies and other media can multiply the entries representing a document (so that the work above might get four separate entries, say, under Stomach, Cancer, Diagnosis and Radiography) this option is not open for the physical arrangement of the documents; a document can go

in one place only. If the library user is to locate any given subject class easily, the sequence of classes throughout must reflect strict rules for the combination order (citation order) in such classes. So the work above might be located as: Stomach - Cancer - Diagnosis - [using] Radiography, and nowhere else. Applying such rules minimizes the central (but unavoidable) weakness of the linear order, which is the scattering of some concepts by subordination to others (as works on cancer will be scattered under the different parts of the body in the order suggested above).

**1.5** While the development of such rules is a necessity if the location of any given class is to be predictable, it is also the great strength of library classification as an instrument in retrieval. The demands made by the need for comprehensive rules for a consistent order of combination force the designer of the classification to examine closely the categories into which the many concepts fall, and the multifarious relationships between them, more rigorously than is the case with any other system of retrieval. The exposure of synonymity or near-synonymity between terms is only one by-product of the rigorous mapping of the semantic (generic and partitive hierarchical) and syntactic (non-generic) relationships between them. As a result of that analysis the modern faceted classification is the most comprehensive and sophisticated organization of knowledge to be met with in the field of information retrieval.

**1.6** The detailed Outline on page 1 (after the preliminary pages) is designed to give a clear view of the basic structure of Class C. If it is remembered that the schedule is an inverted one (see Section 7.22) the outline will be seen to show not only the general sequence of categories and their classes but also the basic operational rule in applying the classification. This is the rule that compound classes (those reflecting the intersection of two or more simpler classes) are located under the class appearing later (lower down) in the schedule. For example, the class Allotropes of selenium CMR GQ is located under CMR and not under CGQ, since CMR files later in the schedule than CGQ.

## 2 Scope of Class C and its place in BC2

**2.1** A general discussion of the sequence and relationships between the natural sciences may be found in the introduction to Class AY/B, General Science and Physics (3). The order of main classes in BC2 reflects as far as possible the Comtean principle of gradation (as Bliss called it), which finds a parallel in the more recent theory of integrative levels. The latter suggests that there is a natural order of systems in the broadest sense, more complex systems emerging from, and dependent on, simpler systems (4); it provides an appropriate basis for the ordering of main classes, or disciplines, in bibliographic classifications (5), and closely parallels Bliss's own ideas of main class order, generally regarded as the best and most carefully argued of all the general schemes. This views Physics as dealing with the fundamental concepts of energy and matter at the subatomic level (at which the two concepts may become interchangeable), and Chemistry as dealing with the forms of matter at the level of atoms, ions, molecules and molecular systems, together with the energy relations between these.

**2.2** This division of the two fundamental sciences seems to work quite well, both logically and practically, reflecting, as Bliss would have said, the scientific and educational consensus which governs the division of labour in these fields. However, Vickery (6), in a pioneering paper on the application of facet analysis to chemistry, suggested that 'a more logical place to put the protons, etc., is in the substance facet of Chemistry, which would then be better entitled, the Science of Substances. But it may be that logic should give way to tradition.' As it is, the general class for subatomic particles in BC2 is Class B Physics, and this is available to be drawn down under Class C Chemistry whenever the occasion demands (which is very often). There seems to be little doubt, however, that the literature on a concept like electronic orbitals, say, which are so critical in determining the structure of and interactions between atoms and molecules, belongs to chemistry, since the more highly organized level of these is clearly implied.

**2.3** Because of its fundamental nature, the subject matter of chemistry appears at many other levels of the general classification. One major example of this is mineralogy, which deals with naturally occurring molecular aggregates in an implied terrestrial context; this is collocated with the earth sciences in Class D. Another is biochemistry, which deals with chemical substances and reactions defined by the context of living organisms. At a yet higher level, these substances and reactions may appear in the context of particular organisms, including humans; here they constitute a large and important field in their own

right, in which they are crucial factors in normal anatomical and physiological matters, as well as appearing as agents of disease and of diagnostic and therapeutic action.

## 3 Structure of classes in BC2

**3.1** All classes in BC2 are designed consistently according to a basic pattern which displays the fundamental components of a modern documentary classification. In the design process these components are addressed in an invariant order in which each step depends on the preceding ones. The steps are, in order:

**3.11** Organizing the terms into broad facets.

**3.12** Organizing the terms in each facet into specific arrays.

**3.13** Deciding citation order (between facets and between arrays).

**3.14** Deciding filing order (of facets and of arrays).

**3.15** Adding notation.

**3.16** Adding an alphabetic index.

**3.2** The theory underlying these features is explained in detail in the Introduction to BC2 (2), in chapters 5 and 6. Here, in this introduction to Class C, the structure and fundamental features of the class are described in the order of the six steps above, and it is assumed that users of this class will familiarize themselves with the essentials of the theory explained in the Introduction to BC2 as a whole.

## 4 Facet structure of Class C Chemistry

**4.1** The main feature of the schedule is a strict adherence to the principles of facet analysis. A facet is defined as the sum of classes produced when the vocabulary is divided by one broad principle of division. So the terms making up the vocabulary of chemistry are initially organized into ('divided into') broad facets; terms representing concepts which all stand in the same broad relationship to the containing class are found in the same facet. For example, all terms reflecting the notion of a type of substance (e.g., element, compound, carbon, carbon monoxide, acid, alcohol, liquid, coordination compound, condensation product) are brought together in a Substances facet. All terms reflecting a chemical process (e.g., reaction, addition, substitution, phase transformation) are brought together in a Processes facet. All terms reflecting some external action (usually by chemists) such as analysis, detection, weighing, and separating, are brought together in an Operations facet, and so on.

**4.11** Facets correspond to a set of fundamental categories, which when applied to a given subject domain generate groupings of the kind described above. The categories used in all classes in BC2 are those identified in the work of the United Kingdom Classification Research Group (CRG), which, during the second half of the twentieth century, developed the faceted classification theory of S. R. Ranganathan. These categories may be summarised as: thing (or entity); kind; part; material; property; process; operation; agent; product; by-product; time; and space. These have been found to accommodate the terminology of all the classes worked on so far, although not all categories are necessarily represented in every subject. The methodology is particularly appropriate to the domain of chemistry which has a strong formal structure, and a clear and largely unambiguous vocabulary.

**4.12** Methods of constructing classification schemes are often referred to as 'top-down' or 'bottom-up', depending on whether the subject domain is subdivided hierarchically into a series of classes and sub-classes, or whether the structure is assembled from its constituent concepts. In the case of BC2, although the terminology is 'divided' by the broad principles of division, in practice the facets are assembled by aggregating concepts that share facet attributes (such as 'process' or 'entity'). The methodology is thus a hybrid one, and it is firmly rooted in the terminology of the domain.

**4.2** The facets identified in Class C are summarized below; their scope and relations are considered in more detail under citation order (Section 6).

**4.21** Substances. This facet includes, for example, elements, compounds, metals, hydrogen, salts, binaries, gases, addition compounds, catalysts, allotropes, lithium, nucleotides, adenine triphosphate.

**4.22** Parts. Most of the terms in this very large category may also be regarded as substances in their own right and are not distinguished as parts (e.g., radicals, functional groups, atoms within a molecule, subatomic particles, monomers, surfaces).

**4.23** Processes and properties. Although Property is conceptually a distinct facet (and is sometimes defined as a conceptual or abstract Part) it is in practice difficult to distinguish from processes within a substance (e.g., electronic configuration, temperature). In practical terms, the vocabulary of this facet reflects all those concepts which collectively make up physical chemistry, and the facet includes thermodynamics, stoichiometry, stereochemistry, reactions of all kinds, and change of state.

**4.24** Operations. Operations differ from processes in being actions performed externally on substances and include all the procedures found in practical and preparative chemistry (laboratory techniques, heating, cooling, weighing, transferring, and so on). Its biggest single class is chemical analysis.

**4.25** Agents. This facet includes all those concepts which assist the conduct of operations (e.g., laboratories, equipment and instruments) and in its widest sense it includes also the personnel conducting the operations. But the relationship of Agent is not confined to this general level and may occur anywhere in the Properties and processes facet; for instance, chemical reagents and catalysts are agents.

**4.26** Common subdivisions. These are concepts found in virtually all subjects. In chemistry, they include terminology, information services (abstracts, automated services, etc.) and the history of chemistry (which is the history of the study of chemistry and not the history of the chemical phenomena themselves).

## 5 Arrays within the facets

**5.1** Most facets contain terms which reflect different specific principles of division (while a facet as a whole reflects only one broad principle of division). The terms identified by the application of a specific principle of division constitute an array. For example, in the Substances facet, further division may be specifically by number of elements (to give simple elements and compounds), by atomic structure (metals, non-metals), or by molecular structure in the case of compounds (acyclic, cyclic). It also includes the distinction between inorganic and organic compounds (based on the unique self-bonding characteristics of carbon).

**5.11** Principles of division for particular arrays may also be derived from elsewhere in the classification. For example, various kinds of chemical substances may be characterised by a physical or chemical process or a property (e.g., covalent compounds, electrovalent compounds, conductors, luminescent substances, catalysts, gases). The property or process involved is known as a specifier (literally species maker), and the array is usually designated as, for example, ‘kinds by x property’.

**5.2** Successive levels of division occur all through the classification. For instance, the appearance of organic cyclic compounds introduces a number of arrays peculiar to that class; these include the number of members in the ring (size of ring), and the number of rings in a given compound. If there are two or more rings, the class thus generated (polycyclic compounds) generates yet another set of arrays: the specific number of rings (bicyclic, tricyclic, etc.), the elements making up the ring (homocyclic or heterocyclic), and so on.

**5.3** Terms in an array are mutually exclusive, so there is no problem of compounding between them; there is no class of monocyclic bicyclic compounds, for example. So the crucial problem of citation order (see Section 6) no longer arises within arrays, only between them.

## 6 Citation order (combination order)

**6.1** This refers to the order in which the elements of a compound class (one consisting of more than one element, whether from different facets or from different arrays) are combined (or cited) in a heading; for instance, whether a heading should be:

Chemical analysis – Compound X, or
Compound X – Chemical analysis

When a class has three or more components, the possibilities multiply rapidly. For example the class: Heterocyclic compounds – Monocyclic – With five-membered ring – With mixed heteroatoms – Nitrogen and sulphur, would allow five different citation orders, even if we assume the first component (heterocycles) will remain first in order. Within the class Heterocycles there would be 120 different ways of combining the five different components (the factorial product of five).

**6.2** Citation order reflects the order of application of principles of division and determines which concepts are subordinated to others. For instance, in the first example (Analysis of compound X) the first order would scatter material on compound X while keeping together all the material on analysis; the second order would keep material on the compound together at the expense of scattering material on analysis.

**6.3** The result of a consistent citation order is that the scattering of some subjects because of their subordination to others (a major and inevitable feature of bibliographic classification applied to shelf order, or to catalogues and bibliographies) is strictly controlled and the location of quite complex classes (reflecting several facets or arrays at the same time) is always predictable, and the retrieval of the information on those classes ensured. Citation order is the most important feature of a classification system, or indeed, of any other pre-coordinated knowledge organization system, such as a subject heading list. But clear and consistent rules for it can only be expressed in terms of the facets and arrays involved; hence there exists the prior need to organize terms into their facets and arrays.

**6.4 Citation order between facets**

**6.41** In all its classes, BC2 seeks to observe as far as possible the standard citation order between facets established by the CRG. This takes as the primary facet (the first-cited one) that facet which reflects the ultimate purpose or object of study and is its defining feature. This is then divided successively into:

1. Its kinds, or types.
2. Its parts, subsystems.
3. Processes within it.
4. Actions, external operations on it.
5. Agents of actions.
6. Place (a common facet).
7. Time (a common facet).
8. Bibliographical form, vehicle of information.

Properties of any concept are subordinated to that concept, whatever category it belongs to (part, process, etc.). Common facets (place, time, and so on) are usually cited last. Apart from pragmatic considerations of which aspects of a subject should be prominent (on the whole user expectations will be that information relating to substances should be collocated rather than scattered), the standard citation order reflects a principle of dependence; parts of an entity are dependent on the entity's existence, for example, and an agent of an action presumes the action, and the action presumes the entity on which it acts).

**6.42** The following notes explain how these general rules have been applied to Class C Chemistry.

**6.421** The primary facet is that of Types of substances. These define the subject and are the overall systems within which all other chemical phenomena (processes and properties, etc.) manifest themselves.

**6.422** The second-cited facet is that of Parts of substances. It was noted in Section 4.22 that in practice these are rarely distinguished in chemistry from the types of substances themselves. But in relation to other facets the category of Part is fairly prominent (e.g., parts of equipment in practical chemistry).

**6.423** The third-cited facet is that of Processes and properties. These all imply a containing substance or part of a substance. When a concept is clearly distinguishable as a property as distinct from a process, the property is cited after the process. Properties have an exceptional status as a facet in that anything,

abstract or concrete, may display properties (even properties themselves) and since they depend on that to which they belong they are always cited after it.

**6.424** The fourth-cited facet is that of Operations, reflecting the principle that actions on anything are subordinated to the object of the action (so that the analysis of a given compound, for example, is subordinated to the compound). Operations are distinguished from processes as being external to the object, while processes are internal, a part of the behaviour of the object.

**6.425** The fifth-cited facet is that of Agents, defined as anything which enables or assists an action (process or operation).

**6.426** The last-cited facets are the common facets (common subdivisions); these include concepts relating to the form of presentation of information (such as tables, abstracts, dictionaries, and so on).

**6.43** For the great majority of compound classes the process of combining the elementary terms is a retroactive one, starting from the term filing latest in the schedule and adding to it terms filing earlier. An important exception to this occurs when a given concept appears in a relationship different from its normal one in the general class. The commonest situation is when a substance features as an agent of an operation (e.g., as a reagent in a given test). In this case, that substance is no longer the ultimate object of study, but is acting as something which assists the operation of the test; the ultimate object of study here is the substance being tested. The first title in Section 12.7 (on practical classification) is an example of this situation. It should be noted, however, that the basic relationships postulated by the standard citation order as giving an order of maximum logicality and helpfulness, are still being observed, for instance in the subordination of agents to the actions they serve.

### 6.5 Citation order within facets (between arrays)

**6.51** Apart from Ranganathan's principle of decreasing concreteness, which is of limited application, there are no general principles as yet available for deciding citation order between arrays. Decisions are largely pragmatic, based on consideration of where any given compound (reflecting two different arrays) would most helpfully go.

**6.52** The principles operating in the standard citation order are still applicable to a limited extent in deciding citation order between arrays.

**6.53** In order to maintain maximum consistency in the subdivision of any class of compounds, those types specified by preceding facets are cited after those special to the class (for instance, at CO Organic compounds, classes COG/COI J are cited after those in COI X/CS).

**6.54** The number of different arrays is so large that it is out of the question to list them in citation order as is done for facets in Section 6.4. However, the order in which they should be cited is shown clearly by the inverted filing order (see Section 7); an array filing later (further down) in the schedule should be cited before one filing earlier. An example of this is shown in Section 9.4 below.

## 7 Filing order

**7.1** This is the order in which the individual classes, simple or compound, file one after the other, whether in the schedule, on the shelves or in a catalogue or bibliography. The difference between filing order and citation order is seen very clearly in the telephone directory, where the filing order of headings is alphabetical but the citation order is one of Surname - Forename. In BC2 it has two quite separate components, facet filing order and order in array.

### 7.2 Facet filing order

**7.21** This is the order in which the individual facets (each one containing a block of different classes) file one after the other.

**7.22** The schedule is an inverted one; that is, the facets file in an order which is the reverse of the order in which they are cited when terms are compounded. So the primary facet (Substances) files last, the second-cited facet (Parts) files next to last, and so on.

**7.23** The reason for this (explained more fully in the Introduction to BC2, Section 5.742) is solely to preserve a consistent general-before-special sequence of classes. For example, in Section 7.25 below, the class Bonding at CAG is bonding in general and covers all substances; at CQA G it has narrowed to bonding in a particular category of compound i.e. it is more special, or more specific in scope, than CAG. It files after the latter because the Substance facet files after the Properties and processes facet. This principle ensures that the compound concept of 'Bonding in cyclic compounds' does not file before either 'Bonding' or 'Cyclic compounds', both of which are more general in nature, and thus preserves the general-before-special rule.

**7.24** Similarly, within each facet the arrays are inverted; the first-cited array files last, the second-cited array files next to last, and so on. For example, at CS Heterocycles, the first-cited array (By number of members in the ring) files after the second cited (By heteroatom).

**7.25** It was noted in Section 1.6 that the inverted filing order embodies within itself a comprehensive guide to the citation order. The sequence of classes below demonstrates this:

| | |
|---|---|
| C | Chemistry |
| | . (Processes and properties) |
| CA | . Physical chemistry |
| CAG | . . Bonding |
| CG | . (Substances) |
| CIA | . . Acids |
| CQ | . . Cyclic compounds |
| CQA G | . . . Bonding in cyclic compounds |
| CQI A | . . . Cyclic acids |

The above sequence, from which many classes have been omitted, of course) implies, inter alia: firstly, that a substance is cited before a process or property; secondly, that between the arrays in the Substances facet, the array of compounds by structure are cited before the acid/base/salt array.

### 7.3 Order in array

**7.31** The classes in an array are mutually exclusive and cannot normally be compounded, so their filing order cannot be determined by citation order. Where there is an obviously helpful order, it is used, as is numerical order, in the number of rings in polycyclic compounds, and the range of different valencies in some elements. Alphabetical order is sometimes the best way to handle a large and indeterminate number of classes in an array. In other cases, the order is pragmatic.

## 8 Alternative locations and treatments

**8.1** Alternative locations and/or treatments are provided for in a number of cases, and the notation has been designed specifically to allow alterations to be made to the preferred arrangement. In all cases, the preferred arrangement is stated clearly, and any special notational instructions needed to implement the alternative are indented under the note for it, to stress its subordinate status.

**8.2** The general pros and cons of alternatives are explained in the Introduction to BC2 (2) (Sections 5.744, 6.22 and 6.344).

**8.3** The main alternatives in Class C are these.

**8.31** The most far-reaching one is the provision for locating Process engineering (Chemical technology) at CX/CY. The reasons for the separation of technology from the natural sciences in BC2 are referred to briefly in the Introduction to Classes AY/B (3) (in Section 1.3), and in the Introduction to Class U/V Technology (currently in draft format).

**8.32** Almost as far-reaching is the provision for the collocation of the special classes of organic chemistry at CTH/CW. These are considered in more detail at 11.7 in the section on special problems in Class C.

**8.33** Mineralogy may be located at CFX (following chemical crystallography), although it is preferred in Class D with petrology and soil science at DIP. This also is considered further in section 11.72.

**8.34** Alternative treatments are sometimes distinguished from alternative locations; this happens when the general location of a class is undisturbed but a different way of handling a particular type of subclass is provided for.

## 9 Notation

**9.1** The notation is purely 'ordinal', that is, it makes no attempt to express hierarchical relations by adding another letter or number to symbolize each step of division. Such an attempt must always fail sooner or later (more likely sooner). So BC2 notation concentrates on the primary function of notation, which is simply to maintain the order of classes already determined completely by the theoretical rules governing order (citation order and filing order). By doing this, it secures classmarks which are as brief and as simple as possible.

| | |
|---|---|
| CQ | Cyclic compounds |
| CQA | . Physical chemistry |
| CQA O | . . Molecular structure |
| CQA P | . . . Stereochemistry |
| CQA S | . . . . Symmetry |
| CQA SS | . . . . . Centre of inversion |
| CQA T | . . . . . Reflection symmetry |

Only four classmarks in the above chain (sequence of successively subordinate classes) are 'hierarchical' in that they add characters to the classmark of their immediate containing class; CQA, CQA O, and CQA SS are 'seen' to be subordinate to CQ, CQA, and CQA S respectively. On the other hand, the classmarks are shorter than they would have been otherwise; the last class would need a classmark at least eight characters long if the notation were hierarchical.

**9.11** It also follows from the general rules for building classmarks for compound subjects (described below) that the resulting notation is not expressive of the facet make-up of the subject. Since there are no facet indicators, and shared letters are dropped, the notations for individual components mutate during the process of combination, and are obscured in the final classmark. While this is not significant for organization in a linear file it does have some implications for machine handling and retrieval using BC2 classmarks, and is a problem that will need addressing in the future.

**9.2** The notation is fully faceted and synthetic. Compound classes formed by the intersection (coordination) of two or more separate concepts or classes are given classmarks which are built ('synthesized') from the simpler constituent classes according to strict rules. These are explained fully in the Introduction to BC2 (Section 7.4), but the essential ones are repeated here for convenience and the easier understanding of the notation in Class C, which has some distinctive features.

**9.3** The chief method of synthesis is by direct retroactive notation. As a general rule, for any given class in the schedule all those preceding classes (belonging to different facets or arrays and therefore potentially combinable with the class) are available to qualify it by adding the earlier classmark minus its initial letter (in this case, C) directly to the classmark concerned. For example:

| | |
|---|---|
| C8E | Preparative chemistry |
| C8K R | . Phase separation concentration |
| CAY | Reaction chemistry |
| CB | . Physics of reactions |
| CBA T | . . Transport processes |
| CCD B | . Reversible reactions |
| CDS | . Mechanochemistry |
| CF | . Mixed phase chemistry, phases (reactions) |
| CF8 KR | . . Phase separation concentration |
| CFB AT | . . Transport processes |
| CFD S | . . Mechanochemistry |
| CFF | . . (Processes in change of state) |
| | . . . * This is the first enumerated subclass of CF. |

CFF R . . . Phase transition
CFF T . . . . Phase equilibrium

The fact that the special divisions of CF begin only at CFF means that all the classes preceding CF may be 'added' directly to CF (minus their initial C) without clashing with the enumerated subclasses special to CF, which begin at CFF.

**9.4** Clearly, direct retroactive synthesis requires that all the letters introducing facets and arrays earlier than the class being qualified must be 'reserved' under the latter, so that the first subclass special to it (its 'first enumerated subclass') must be given a letter later in the alphabet than all those preceding the class. As classes begin with later and later letters of the alphabet, so the number of earlier letters to be reserved increases, and the letters available for enumerating the special subclasses decreases. This presents no problem to a purely ordinal notation, because the next 'notational array' is drawn into service to accommodate these further special subclasses.

CQ Cyclic compounds
. (By number of rings)
CQQ A . . Monocyclic
. . . * This is the first enumerated subclass
. . . . of cyclic compounds (a very large class).
CQQ B . . Polycyclic
. (By special bond structures)
CQX . . Alicyclic, non-aromatic compounds
CQY . . Aromatic compounds
CR . . . Benzene
. . . . * Add to CR letters A/MP following CQ;
CRQ B . . . . Polycyclic benzenes
CRQ E . . . . . Bicyclic
CRQ EN . . . . . Naphthalene
CS . Heterocyclic compounds

That CR, for example, doesn't 'look like' a subclass of CQY, or that CRQ EN doesn't look like a subclass of CRQ B is of no consequence in a purely ordinal notation. The classmark CRQ EN performs its essential function (of locating the class Naphthalene in relation to tens of thousands of other classes) precisely and economically. Similarly, the very large class of aromatic compounds is not restricted to CQY; the retroactive classes A/MP (from CQA/CQM P) are added to CR (A/F having been added directly to CQ from CA/CF), so that shorter classmarks are gained for the bulk of the literature.

### 9.5 Adding classmarks from preceding arrays

**9.51** In many cases two classmarks that are linked have two initial letters in common. As a rule, both these letters may be dropped when adding earlier classes.

CF . Mixed phase chemistry
. . (Kinds by number of phases)
CFL . . . Homogeneous chemical systems, single phase systems
CFN . . . Heterogeneous chemical systems, multiple phase systems
CFN T . . . . Dispersions, disperse systems
. . (Systems by pure state of matter)
CFS . . . Fluids
. . . . (Kinds by complexity)
CFS L . . . . . Homogeneous
CFS N . . . . . Heterogeneous
CFS NT . . . . . Dispersions

In the last three classes the letters CF, common to CFL, CFS, CFN and CFN T, have been dropped.

**9.52** Not infrequently it would be quite feasible to drop the initial three or even more letters when adding arrays within the same notational facet. A special instruction is usually given when this occurs.

### 9.6 Intercalators

**9.61** Another method of synthesis found often in Class C is the use of a particular letter (or number, sometimes) to 'introduce' or indicate a set of classes inserted at a required point in the schedule. The selected letter or number is called an intercalator. The chief situations in which this occurs are these.

**9.62** Earlier classes are used to specify types of something. An example of this is at CGH G where processes and properties (whose normal role is to qualify the substances which follow them in the schedule) are used instead to specify (i.e. define species of) those substances. The notation for the earlier classes (CAA/CAW) is added to CGB/CGD or to CG for substances.

**9.63** One class is amplified by another class in C, but outside the normal retroactive system (see Section 6.43). For instance, at CG Substances, notations for comprehensive works on individual elements are got by adding to CGF classmarks from the later array at CK/CNY, to give, say, CGF NQ Cobalt, from CNQ (see also Section 9.66 below).

**9.64** A class or part of a class is amplified from outside Class C. One prominent example of this is at CAB Physics of chemistry, where the terminal B is an intercalator allowing the insertion of the complete physics class B. This provision is repeated at CB Physics of reactions, in order to allow a shorter notation for a prominent application of physics to chemistry.

**9.65** Interruption of normal retroactive notation is sometimes resorted to in order to secure a shorter classmark for an important class. An essential feature of interruption is that it always maintains the overall systematic order and accounts for every single class that normal retroactive synthesis would provide. This example demonstrates the provision of a brief classmark for Ammonium, while preserving the logical sequence of classes:

| | |
|---|---|
| CLS | Nitrogen |
| CLS IE | . Salts |
| K | . Compounds with hydrogen |
| KJ | . . Nitrogen hydrides |
| KJH N | . . . Trivalent |
| | * Normal retroactive notation is interrupted here in order to give short classmarks to ammonia and ammonium. It is resumed at CLU. |
| M | . . . Ammonia |
| CLT | . . . Ammonium |
| CLT IE | . . . . Salts |
| LMM | . . . . Ammonium compounds with carbon & oxygen |
| CLU | . . Other compounds of nitrogen and hydrogen |

### 9.66 Non-retroactive classmark synthesis, building forward

**9.661** A major provision found necessary in Class C is one in the Elements array (CJW/CNY in inorganic chemistry, COM X/COP Y in organic chemistry) for building classmarks forward as well as retroactively. This is caused by the unreliability of chemical formulae as a basis for citation order between the elements in a compound and the need to fall back on the retroactive principle in many cases. Consequently, each and every element has the notation for the complete range of elements reserved under it to allow both forward and retroactive synthesis. The notes at CJW should make this clear.

### 9.7 Enumeration of compounds in schedules

**9.71** In principle, a faceted classification consists simply of facets and arrays of relatively elementary terms; all compounds are formed by the classifier, who assigns classmarks to them by means of synthesis, observing strict rules of citation order. This is a very economical way of presenting the classification, as was shown by the very first faceted classification to be made (Ranganathan's Colon Classification) (7).

Since the exact location of all potential compounds was fully predictable it was thought unnecessary to enumerate them in the schedules.

**9.72** This principle is considerably modified in BC2. For instance, when a synthesized compound has its own particular name or names, which clearly should appear in the schedule, and in the alphabetical index, the compound cannot appear unless its classmark is given to show its exact location. Usually the term signifying the general concept in its original facet or array is added to make clear the context defining the compound.

```
CDU GQ      Heat of reaction
CDU GR      . Heat capacity
            . . Measurement
CDU GR7 6   . . . Calorimetry
```

This enumeration also prevents the general facets or arrays from being swollen by numerous terms that are not truly general.

**9.73** More important than these specific situations is the general aim of BC2 schedules to appear as clear and informative to their users as possible. This is often achieved by bringing down prior, more general classes, in order to locate specifically a particular subclass in its exact hierarchical position. Since all classification is definition this assists the users (the indexers) to understand exactly what is happening in a situation with which they may not be completely familiar. It also assists interpretation of and familiarization with the synthetic classmarks, which can become somewhat daunting when the class is highly specific. The locating of specific heterocyclic compounds in class CS is probably the most detailed of these presentations.

**9.74** The extensive elaboration of the schedules just noted has proved particularly necessary in chemistry. Vast numbers of compounds exist that potentially demand recognition because literature appears on them, but those compounds that are enumerated can be only a small fraction of the total, which in any case is constantly growing. It is therefore essential that sufficient detailed structure is provided for the indexer to locate with some exactness where any unlisted compound goes.

**9.75** This expansion of the schedule has the additional advantage of expanding the core terminology, a process which is vital where it may form the basis of a thesaurus or other controlled vocabulary (see Section 13). Compound terms of the kind ‘Bond strength in transition metals’, which evidently combine two simpler concepts would not normally be included in a thesaurus. However, terms such as ‘hydrides’, ‘borates’, ‘carbonic acid’, and ‘chlorobenzol’, all of which represent combinations of simpler concepts, certainly would. It is only by pre-coordinating these concepts, and locating the compound in the correct place in the schedule that they are properly represented in the terminology.

**9.76** When some enumerated compound classes appear in the schedule, it should not be thought that the detail there is limited to those subclasses enumerated. When you look at the specificity of the vocabulary in a given class, always remember that the class may be qualified by all earlier facets, whether this is hinted at by a limited enumeration or not.

**9.8** The different ways of building classmarks described above may give an impression of complexity at first reading, but so would the simplest action if described in terms of its basic operational steps. Applying notation is a practical operation. The steps involved are basically simple and quickly become familiar after a little practice. Detailed explanations and examples are given in the Introduction to BC2 (Section 7.4) and a simple flowchart covering all possibilities appeared in the Bliss Classification Bulletin for January 1978.

## 10 Alphabetical subject index

**10.1** The function of the alphabetical index in a classified indexing system is considered in the Introduction to BC2 (2); Section 6.5 there gives the general principles used in BC2, and Section 7.5 gives practical guidance to a library making its own alphabetical index to its own stock.

**10.2** The basic points to be remembered for efficient use of the printed index to the schedules of this class will be found on the page preceding the alphabetical index.

**10.3** The basic rules of this index are those of chain indexing. If an entry is qualified at all, it is by a superordinate class (which helps to define it). An entry term is never qualified (followed by) a term representing one of its own subclasses in the schedule. For instance, the entry:

Organic compounds CO will appear, but not the entry:
Organic cyclic compounds CQ

The latter will have its own entry under Cyclic compounds: Organic, in which the qualifying term (Organic) represents the containing class, defining what the Cyclic is referring to.

**10.4** The alphabetical index to Class C has been produced largely by automatic selection of terms from the schedules, and the program includes rules for deleting 'anti-chain' entries. Entry terms are qualified only when the same entry term leads to more than one classmark and it is necessary to distinguish the context of each. The index has not been manually edited, so some of the entries are inelegant in format; it is hoped that these deficiencies will be overlooked by users.

## 11 Special problems of classification in Class C

**11.1** So far as is feasible, problems of definition and analysis and the practical decisions taken to meet them are noted in the schedules at the point of application. Others are implicit to some extent in the provision of alternatives. But a number of theoretical problems seem to call for more extended consideration, and that is the reason for this section.

**11.2** The most significant problem in chemistry is the enormous number of concepts in the primary facet of Substances. It is hard to determine a precise figure for the number of chemical substances known, partly because the basis for counting is not easily established. The CAS Registry, a division of the American Chemical Society, and the official body for recording new substances and allocating registration numbers, had 67,246,263 records at the time of writing; this figures changes by the second, and CAS add 15,000 new items every day (8). However, their databases include reactions and synthetic procedures as well as substances, and a more conservative figure, generally agreed by reference sources, is 12 million, growing by approximately 100,000 annually. The scale of this places chemistry on a par with biological sciences in terms of the number of entities to be organized, but in chemistry the problem is exacerbated by the lack of standard classification systems for substances. Although some classifications exist, they tend to be for fairly specific groups of chemicals, such as drugs, or hazardous substances, and the structure of the classification is usually based on some non-chemical principles, such as practical the management of the materials or the law relating to them.

**11.3** The problems of taxonomy are separate from, but not unrelated to, those of the description of chemicals and their representation. Chemical nomenclature is a significant study in its own right, and one of the major features of the discipline is the proliferation of names of all kinds: popular and trade names, as well as the properly scientific, the latter regularly taking variant forms. Chemistry again fares badly in comparison with the biological sciences, there being no widely accepted standard rules for naming. The one general system for standardization is that of IUPAC (the International Union of Pure and Applied Chemistry), in which IUPAC aims to relate the name of a chemical compound to its structure, and hence to its molecular formula (9). Names of inorganic compounds include the various ions and an indication of valency, as well as the hydration state. Guidelines for the naming of organic compounds resemble the Linnaean system for biological organisms, describing any compound in terms of its parent hydrocarbon (the length of the underlying chain) and its parent functional group. For more complex compounds, to this are added the names of any side chains, additional functional groups, and, where appropriate, their location on the chain, and the presence of double and triple bonds. The whole is controlled by a strict citation order, and includes numbers as well as descriptors for the various structural elements. While this provides an accurate name for any particular compound, the names produced are often not immediately familiar, and it is not necessarily adhered to in practice. Neither is the approach necessarily the best basis for selecting names for subject indexing purposes

**11.31** Class C has adopted no particular comprehensive policy on the forms of names, and the captions for classes sometimes contain popular names (such as 'quicklime' or 'milk of magnesia') as well as traditional names such as 'wolfram'. These are not normally the preferred form of name, and do not take the lead position in the class description, although they do feature in the index. More narrowly scientific names for chemicals can take various forms and these are routinely represented in the schedules (for example, magnesium bicarbonate, and magnesium hydrogen carbonate).

**11.32** A useful reference tool in the identification of names is the Merck Index, an encyclopaedia of chemical substances, which brings together the different forms of name for chemical compounds, listing trade names and popular names, as well as more structurally descriptive names (10). This has been invaluable in reconciling varieties of name, and imposing some control on the BC2 vocabulary.

**11.33** The various published standards have been used as a guideline in the exclusion of some older names, and where a term does not appear either in the Merck Index, or the IUPAC documentation, it has normally been omitted. IUPAC has also provided an authority for the names of newly created super-heavy elements, acting as an indicator of international agreement. The National Library of Medicine's Medical Subject Headings (11) have been consulted as an external authority in respect of the biologically important substances. Some attention has also been paid to the occurrence of names in the scholarly literature, and where a name has not been used for some decades it is unlikely to be retained.

**11.34** Allied to matters of nomenclature is the question of how far the molecular formula should be notationally encoded. The discipline of chemistry has produced several notational schemes of this kind, the original and most well-known of which is probably Wiswesser Line Notation (WLN) (12), but more recent examples such as SYBYL (13) and SMILES (14) have been developed. These representation languages are particularly useful in chemical database work, but not appropriate at all for conventional classification and indexing. In theory, the classification codes in BC2 might be used in a similar way, although the non-expressive nature of the notation would be a barrier. But the most significant argument against it would be the requirement to make the classification structure exactly mirror the chemical composition of compounds, and this is not feasible in a bibliographic classification such as BC2.

**11.4** Scientific naming, however systematic, does not in any event provide an answer to the problems of bibliographic classification, which must accommodate works on general classes of substances, as well as specific individuals. As in other disciplines which require a 'taxonomic' classification of entities as the primary facet, Class C requires detailed analysis of the various attributes of substances, including functional and structural properties, since these attributes supply the principles of division for the arrays which constitute the taxonomy. This means that numerous classes of structures found among chemical compounds, especially in organic chemistry, have to be incorporated in the classification before the specific compounds can be located. Therefore the greatest problem by far has been the working out of the detailed schedule for the primary facet of substances. To take only one array, though it is the central one, that of compounds defined by their constituent atoms: although the number of elements is only ninety or so, the number of compounds which potentially call for recognition is enormous. While all these structures reflect particular relationships between the same limited number of constituent elements (e.g., the number of rings in a polycyclic compound, the constituents of those rings, their mode of linkage) they introduce factors for which even the fully structural formulae (which may require two- or even three-dimensional graphic presentations) give only limited help.

**11.41** A bibliographic classification like BC2 needs not only to recognize all the numerous arrays within this facet but also to decide a comprehensive citation order between them. A useful clearing of the ground is effected by the well-established principle in faceted classification that, within any given class, those subclasses specified by preceding processes, properties, operations, etc. file before (and are cited after) those classes special to the class being divided. So classes CG/CH are cited after any compounds defined by constitution.

**11.42** In the primary array (compounds defined by their constituent elements) the major distinction between inorganic and organic chemistry comes with the appearance of the element carbon. Organic compounds are defined by the unique self-bonding characteristics of the carbon atom. The fact that it is not treated

as a special set of subclasses following CLM Carbon (where it appears in the sequence of elements in their periodic table groups) simply acknowledges the well-established division of the subject into inorganic and organic chemistry. The latter is invariably treated as a separate class and contains the great majority of known compounds.

**11.43** With organic chemistry comes the concept of basic structures, in which the molecular shape (whether a straight chain or a ring) is the major principle of division. The concept of basic structures (which is scarcely mentioned as a concept per se in most chemical textbooks) is undoubtedly the primary array in a faceted classification of organic chemistry. Its comprehensive classes of aliphatic, cyclic, alicyclic, aromatic and heterocyclic compounds usually form the basis for the presentation of literature on organic compounds. Within these classes, structures special to them will then be cited before specification by their substituent elements.

**11.44** This could be regarded as a logical hiccup, introducing new characteristics of division before the current one, constituent elements, is exhausted (remembering that all organic chemistry is a subclass of the constituent carbon). It arises from the fact that in the new context the molecular structure is a stronger determinant of chemical behaviour than are the constituent elements per se.

**11.45** Another problem of citation order arises from the relationship of basic structures to functional groups. In inorganic chemistry the concept of radicals (the term itself seems to be falling into disuse) clearly reflects the Part category; radicals are defined as groups of elements forming a distinct part of many compounds. They are charged particles and do not qualify as independent compounds. In organic chemistry they are known as functional groups and constitute an important array of their own. Because of their reactivity and the importance they have in determining the behaviour of the compound to which they are attached, they are often used as the basis for the consideration of compounds in textbooks. If this educational consensus (as Bliss would have called it) determined citation order, functional groups would, perhaps, be cited before the basic structures.

**11.46** A further decision was needed about the relationship between functional groups and the elements other than carbon and hydrogen (and to some extent oxygen) that are comparable substituents of compounds within the basic structures. Within the functional groups a relatively limited number accounts for much the greater part of the literature, and this is reflected in their enumeration at COI X/COM P. There, they are classified broadly by their two major constituent elements, the hydrocarbon and oxygen groups. But functional groups may arise from any of the constituent elements of an organic compound and it seems logical to continue the sequence of hydrocarbon and oxygen groups with the rest of the elements in COM T/COP Y (in which their arrangement exactly parallels their arrangement in CJW/CNX). Some textbooks stress the role of these as constituents in organic compounds by calling them heteroatoms, although this usage may be confused with the more usual use of this term as being particular to heterocycles.

**11.5** Within the basic structures, acyclic (aliphatic) and cyclic (homocyclic, alicyclic, aromatic and heterocyclic), the problem of citation order between arrays resurfaces with the appearance of numerous arrays peculiar to the basic structures. In particular, cyclic compounds present arrays based on the number of rings in the molecule, the number of members in a ring (ring size), the mode of linkage between rings, and (in the case of heterocycles) the presence of particular heteroatoms in the ring. At almost every point in the appearance of the resultant classes, further arrays demand recognition; for instance, within polycyclic compounds are found arrays by the specific number of rings (bicyclic, tricyclic, etc.) and by variations in the sizes of the component rings; within heterocycles are found arrays not only by variations in the nature of the heteroatoms but also by variations in their number and in their homogeneity (monoheteroatoms and mixed heteroatoms).

**11.51** The citation order finally decided on for cyclic compounds must be regarded as pragmatic rather than reflecting any fundamental relationships between the different classes concerned. They reflect as far as could be established an approximate consensus on the part of chemists. Since the fundamental citation order among the compounds at large cites the constituent elements first (organic chemistry itself being defined in the first place by its central constituent, carbon) it would seem logical to make the array by

heteroatom the primary array within heterocycles; however, there seems to be a clear preference for treating the size of the ring as the primary array, and this has been followed.

**11.6** The proliferation of different arrays in a class, all of which have a claim to be recognized as an important element in the definition of its subclasses, raises acutely the problem of just how many of the characteristics defining the arrays should be recognized before the enumeration of specific compounds begins. This problem is not confined to the classification of compounds; it occurs also, for example, under reactions (at CB/CE). It is in essence the problem of how far a pre-coordinate faceted classification can go in maintaining specificity, and it is determined in practice by the limitations in length of classmarks deemed tolerable by users. The relative position of every link in the chain of concepts making up the hierarchy has to be maintained mechanically by the notation.

**11.61** BC2 is favourably placed (compared with the other general classification systems) for achieving high specificity, since its ordinal notation can effect large economies in length of notation (see Section 9.1). However, the computerized production of the printed schedules imposes a maximum of eighteen characters for a classmark, and this is probably longer than the criterion of user-acceptability would suggest.

**11.62** The ultimate level of specificity in the Substances facet would be the provision of a unique classmark for each and every compound. The number of compounds makes an extensive enumeration of them out of the question. Moreover, searches of the chemical literature at this level of specificity are well facilitated both by coding systems that identify any compound (Wiswesser, etc.) and by automated services that implement them. So Class C restricts itself to the provision of detailed hierarchies into which any compound can be fitted, and to the enumeration of a limited number of specific compounds, in order to demonstrate as comprehensively as possible how this might be done for any other compounds on which a literature appears.

**11.63** Since specific compounds appear only within well-defined and relatively narrow classes the burden of distinguishing individual compounds is much less than it is for the large formula-organized indexes catering exclusively for compounds of every description. So it is still possible in Class C to individualize any compound completely by adding to the specific class containing the compound a summary statement of the elements present and their respective number of atoms. This is explained in Section 12.5.

### 11.7 Special classes of compounds

**11.71** The problem first appears at CFX, where provision is made (but not recommended) for minerals, as a sort of anterior inorganic substances subclass. Minerals are usually defined as naturally occurring compounds with a characteristic chemical composition, and usually with a crystalline structure. If the general principle of gradation is applied, minerals do not appear until the more special class of planetary systems (and notably the Earth) appears in Class D. Basic constituents of the Earth include rocks in which the main constituents in turn are minerals. BC2 prefers, therefore, to collocate minerals with petrology, at DIP. Support for this view comes from the fact that many dictionaries of chemistry contain only the most cursory definition of a mineral and in some cases fail even to mention the class.

**11.72** Organic compounds display a number of classes which, like mineralogy, historically and practically call for recognition as distinct classes, not to be scattered by adherence to the rules governing the location of the main body of chemical compounds. The classes of compounds at CT/CW, appearing outside the structural hierarchies in CG/CS that could theoretically accommodate them, reflect a special problem in the classification of chemistry.

**11.73** Unlike minerals, these classes are usually considered as part of the general chemical literature. But like minerals, they are all naturally-occurring substances and have a well-developed special nomenclature that reflects the classes within which the literature usually considers them. In addition to the educational consensus that this might be said to show, these classes could claim a special conceptual warrant in that they often show close chemical affinity to other classes in the same position; for instance, peptides show an affinity to proteins, terpenes to both lipids and carbohydrates, carbohydrates to glycosides, and glycosides to nucleosides, and so on.

**11.74** These special classes vary in the degree to which they might be accommodated fairly closely in the general structures of classes CO/CS. For instance, carbohydrates could be located under hydrates of carbon; alkaloids could be treated as a special class of nitrogenous heterocycles; amino acids as acid derivatives of amines. But the variety of structures and constituents within many of them would result in a substantial scattering of their subclasses; a good example of this would be amino acids. If the alternative provided at CON U were used, locating this class in its strict structural context, specific amino acids would be scattered under the different basic structures.

**11.75** Another reason for treating these classes separately, implicit to some extent in the foregoing, is the problem of nomenclature, which is bound up with the definition of particular classes. On this subject one textbook comments: 'Because the IUPAC system leads to rather long and awkward names, a unique system of nomenclature has developed in the field of carbohydrate chemistry' (15), and it goes on to demonstrate the utility of the well-established classes which are generally used. The 1996 IUPAC recommendations for carbohydrate nomenclature (16) includes an appendix mapping conventional names to the IUPAC systematic ones.

**11.8** Analogous to the situation of the special organic compounds is that of chemical technology. The general reasons for the separation in BC2 of the sciences and the technologies (except in the case of biological technologies) are set out in the Introduction to Class AY/I Natural sciences (3) and all of them apply to chemistry. However, in line with general BC2 policy, an alternative is provided at CX/CY for the collocation of chemical technology with chemistry.

**11.9** The arrangement of the elements in CK/CNY raised the problem of which sequence of the different groups of the periodic table should be followed: the well-established and familiar division into two sequences (Groups 1A/8A and Groups 2A/2B) or the apparently simpler single sequence of 1/18 now favoured by IUPAC. The former has the advantage of collocating the S-block and the P-block (often referred to collectively as main group chemistry), while the chief merit of the latter is the greater simplicity of its numbering system. It is a basic principle of BC2 that helpful order (which usually implies logical order) should not be sacrificed to notational convenience. Although the numbering of the groups does not enter directly into the notation of Class C, the analogy seems to be sufficiently close to warrant the decision to prefer the more helpful collocation and therefore to follow the older system (while noting the equivalent IUPAC number in each case).

## 12 Practical classification in Class C

**12.1** The general rules for classifying documents by BC2 are given in the Introduction to BC2 (Section 7) (2) and only a summary of the main points is given here.

**12.2** Decide first which alternatives are to be used (if any) and delete clearly from the schedules those that are rejected. Once this is done it is done for good and henceforth the alternatives are irrelevant to the library concerned. It also results in some simplification of the schedule.

**12.3** Classification deals with the concepts which define the subject of the document and not with the terms used by the author to present those concepts (and which on occasions may obscure the sense of some of them). In disciplines like chemistry this is less of a problem than in, for example, the humanities, since titles tend to be descriptive of content, and terminology is generally precise. Nevertheless, the general point should be borne in mind. The schedule should provide a firm and predictable framework within which the classifier can locate the class (usually a compound class) that accurately summarizes the overall subject of the document, as distinct from any subsidiary subjects referred to in the document.

**12.31** A preliminary to any selection of classmarks should be an independent analysis of the document content. In formulating such a concept analysis the structure of the classification provides some guidelines; it is helpful for the classifier to ask a series of questions in a systematic order, posed in terms of the facets and arrays in their citation order. For example, does this document deal with a particular element or compound? If the latter, is it inorganic or organic? If the latter, is it acyclic or cyclic? If the latter, is it homocyclic or heterocyclic? If the latter, what size of ring? What heteroatom(s)?

**12.32** The questions then proceed systematically through the earlier facets. Is a particular reaction or other process dealt with? Any there any particular property qualifying it? Is a particular operation dealt with, and if so, is a particular agent mentioned? And so on. The checklist of facets and arrays is got easily by working backwards through the schedule.

**12.33** The result of this systematic procedure is a summary statement of the document's overall subject in the form of a chain of terms, such as: Heterocyclic compounds - with six members in ring - Bicyclic - with nitrogen heteroatoms - with two heteroatoms. When the chain is complete, the classmark is built by examining the schedules, and observing the basic rules of retroactive notation and noting any special instructions along the way. The latter are always accompanied by demonstrations and these are usually reinforced by some of the enumerated compounds which follow in the schedule.

### 12.4 Demonstrations of practical classification

**12.41** The procedures for a few titles from recent publishers' catalogues in chemistry demonstrate the general points considered above.

**12.42** Title: Proton conductor solids

The annotation indicates that the object of the work is to consider the role of these conductors in electrochemistry. Examination of the schedule, and adherence to the retroactive rule within the class, give the following chain:

| | |
|---|---|
| CE | Electrochemistry |
| CEG | . Electrolytes |
| | . . (By conductance factor) |
| CEG Q | . . . Protonic conductance electrolytes [enumerated] |
| | . . (By physical state) |
| CEG X | . . . Solid electrolytes [enumerated] |
| | . . . . (By conductance factor) |
| CEG XGQ | . . . . . Protons [from CEG Q] |

and the final classmark is CEG XGQ.

A number of theoretical principles observed in BC2 schedule design are demonstrated by this example:

1. That the chain begins with electrochemistry rather than the general class for solids as substances (CHF V) reflects the principle explained in Section 6.43; here, the solid stands in a process - agent relationship in the context of electrochemical processes, and not a substance - process relationship as in the context of the whole chemistry class.
2. In the chemistry class, the ‘end product’ in electrochemistry is the production of a chemical reaction and so these reactions constitute the first-cited classes (at CEJ/CEP). Electrolytes stand in the relation of agents in this process and therefore are cited after the reactions (and file before them) as components in the process.
3. By the retroactive principle the array filing later is cited before the one filing earlier; in this case, solid is cited before protons.
4. The order of the arrays defining types of electrolytes is consistent with the general citation order in Class C; those defined by constituents (composition) file last, those defined by state of matter file next to last, and those defined by processes and properties file before these (the filing order being the reverse of the citation order in the inverted schedule).

**12.43** Title: Multiple bonds between metal atoms

An annotation makes it clear that this work is specifically on quadruple bonds between transition metals. So the chain is:

| | |
|---|---|
| CJW | Inorganic compounds by specific elements |
| CNA | . D block compounds, transition metals |
| CNA AKS | . . Multiple bonds [from CAK S] |
| CNA AKX | . . . Quadruple bonds [from CAK X] |

and the classmark is CAN AKX.

**12.44** Title: Transition metal organometallics for organic synthesis

An annotation makes it clear that the organometals are being considered as powerful tools in organic synthesis. So the principle explained in Section 6.43 is again invoked and the chain is:

| | |
|---|---|
| CO | Organic compounds |
| COC PB | . Synthesis [from CCP B] |
| COC PB5 X | . . Reagents [from C5X] |
| COC PB5 XO | . . . Organic reagents [from C5XO] |
| COC PB5 XOP A | . . . . Transition metal organic compounds [from COP A] |

and the classmark is COC PB5 XOP A.

**12.45** Title: Field response polymers

The annotation refers to electro-, photo- and other responsive polymers. This suggests that the book deals also with polymers responsive to other fields of the electromagnetic spectrum. So the chain is:

| | |
|---|---|
| CTE | Organic polymers |
| CTE H | . (Kinds of polymers) [from CH] |
| CTE HGB | . . (By mechanics of reactions) [from CB] |
| CTE HGB BH | . . . (Fields of force) [from CBB H (BBH in Physics)] |
| CTE HGB BHO | . . . . Field effects [from CBB HO] |

and the final classmark is CTE HGB BHO.

If a polymer were defined by the electric field responsiveness specifically, the classmark added from B Physics would be BHI BHO, citing the specific field before the effect, and the final classmark here would be CTE HGB HIB HO.

This demonstrates the use of Process/property concepts to define types of chemical substances (provided for at CGH). Note also that the physics concepts are taken from CB since reactions are involved (see note at CAB, which also introduces divisions from Class B for more limited contexts).

**12.46** Title: Asymmetric synthesis of fluoro organic substances

The chain is:

| | |
|---|---|
| CTE | Organic polymers |
| CTG | . (Types by constituent elements) |
| CTG OU | . . Fluoro compounds [from COO U] |
| CTG OUC PB | . . . Formation, synthesis [from CCP B] |
| CTG OUC PBS | . . . . Asymmetric |

and the final classmark is CTG OUC PBS.

## 13 Applications of Class C

**13.1** Two basic approaches can be seen in subject access to information: documents (or other items) can be classified, or categorized, for inclusion in a conceptually arranged scheme, either for browsing purposes, or for retrieval from the shelf; or they can be indexed with keywords or descriptors to indicate content for the purpose of retrieval via the catalogue. The original application of BC2 schedules is to the arrangement of documents on shelves in libraries or other files in linear order, and of entries for them in catalogues and bibliographies. The needs of these applications explain the close attention paid in BC2 to problems of citation order and filing order and to the notation necessary to maintain these in a

mechanical fashion. Information on the construction of catalogues and bibliographies is given in the Introduction to BC2 (2). A very full discussion of these problems will also be found in the Introduction to Class Q (17).

**13.2** The logical and predictable structure of a BC2 schedule is also invaluable as a basis for the construction of other types of subject indexing tools, i.e., those using terms rather than conceptual classes, and to that extent the faceted structure forms a bridge between the two kinds. The comparative ease with which this process can be managed also suggests strongly that facet analysis has a broader and more fundamental role in information organization and retrieval. Matching a concept and its corresponding terms is not a new idea, and Ranganathan writes extensively of the 'idea plane' and the 'verbal plane' as components of classification, as well as the 'notational plane'.

**13.3** The usefulness of BC2 as a source for a thesaurus has been acknowledged for some years, and a methodology for deriving an associated thesaurus is described in detail by Jean Aitchison in a 1986 article (18). In the intervening period this technique has become established as a standard means of constructing a thesaurus (19, 20), and the British Standard for Structured Vocabularies (BS:8723) acknowledges the value of facet analysis as a preliminary to the construction of such vocabularies (21).

**13.31** The thesaurus is essentially an alphabetically organized list of terms used for indexing in a given subject, together with cross-references between the terms that indicate the relationships between them, and allow the indexer to navigate the vocabulary. Vocabulary control is exercised over the terms by the selection of preferred terms from among synonyms ('tungsten' rather than 'wolfram'), and adopting consistent forms of multi-word terms, such as 'inorganic chemistry' or 'bond dissociation energy'. This control reduces the number of options open to the indexer, improves consistency in indexing, and hence makes for more efficient retrieval.

**13.32** A standard set of reference codes, or tags, are used in the great majority of thesauri; these deal, on the one hand, with the relationships between preferred and non-preferred terms (often called equivalence relationships), and on the other, with the hierarchical and other semantic relationships between the terms. These are:

| | |
|---|---|
| UF (Use for) | To link a preferred term to its non-preferred synonyms |
| USE (Use) | To link non-preferred terms to the preferred term |
| NT (Narrower term) | To link to more specific terms in the vocabulary |
| BT (Broader term) | To link to more general terms in the vocabulary |
| RT (Related term) | To link to terms related in some non-hierarchical way |

All of these relationships can be derived from the BC2 structure, either from the class names or from the hierarchy, and with time and patience any BC2 user can construct their own subject specific thesaurus. Detailed instructions for the method can be found in the books referred to.

**13.33** Hypothetical examples of entries in a Class C related thesaurus might look like the following:

Tungsten
- UF Wolfram
- BT Group 6 compounds
- NT Tetravalent tungsten
- Hexavalent tungsten
- RT Chromium
- Molybdenum

Nucleons in chemistry
- BT Particle physics in chemistry
- NT Protons in chemistry
- Neutrons in chemistry
- RT Nuclear physics in chemistry

Oligosaccharides
UF Compound sugars
BT Polysaccharides
NT Disaccharides
RT Homopolysaccharides

**13.34** The strong underlying structure of BC2 is such that it has been possible to adapt the management software to generate a thesaurus, as well as the classification schedules and the alphabetical index. The basic encoding of the BC2 files which controls, for example, the order of classes, levels of indentation, hierarchical display, and the relationship between classes and 'non-classes', such as principles of division, is sufficient for the software to infer most thesaural relationships without any further intellectual input. The main problems occur in the management of equivalence relationships, largely as a consequence of earlier schedules having been compiled without reference to a possible thesaurus format. It is hoped that the introduction of a well formulated editorial policy for the formation of class headings and captions will help to improve the situation, and diminish the need for manual editing. Otherwise, the process has been tested with good results, and it is hoped that in the future we can publish each subject volume as a classification together with an associated thesaurus.

**13.4** BC2 can also be extremely useful in the construction of search aids for automated databases. A very useful account of the problems attending this appears in Chris Preddle's revised edition of Class Q (17). The Introduction to that volume of BC2 considers the problems of subject keyword indexing, the pre-coordination of terms, indexing aids in the control of preferred terms and synonyms, thesaurus construction, and searching for documents by their classmarks. Although the examples given in Class Q are drawn from a field quite different from chemistry, the principles involved are much the same as will be found in any field, and their application to Class Q should be of great help to users of this volume too until an exposition tailor-made for the needs of the sciences, including chemistry, is available.

**13.41** It should be noted that the limitations on specificity that it is necessary to observe in the case of files arranged linearly (Section 11.6) need not be imposed on a faceted vocabulary for searching files not so organized. It is not difficult to imagine this chemistry schedule being expanded so that those arrays are represented that at present are absent from the synthetic hierarchies introducing specific compounds (for instance, under functional groups, the array (By number of substitutions) at COI VJ, and the array (By composition of functional group) at COI VS). Specific compounds would now be defined with maximum precision in the hierarchy which they terminate. An extremely interesting and useful analysis of the problem in chemistry, which takes account of the contribution of faceted classification in automated systems, is given by Robert Fugmann (22).

**13.5** The potential of faceted systems in managed online environments has long been acknowledged, and the appearance of a new range of faceted tools for resource discovery has previously been noted (Section 1.22). The natural affinity of logically structured knowledge organization systems and machine manipulation is self-evident, and facet analysis is increasingly seen as a relevant and effective means of organizing content. A drawback has been the complexity of a fully developed faceted system such as BC2, since most representation languages cannot cope with the complete range of relationships displayed nor with the subtlety of the structural principles. However some considerable progress has been made by the Simple Knowledge Organization System (SKOS) working group of the Semantic Web Consortium which has produced a tool that can represent both standard thesaural relationships, and also some of the features of a faceted classification, such as arrays (23). Friends and colleagues associated with BC2 have been influential in bringing the theory of facet analysis to the attention of the W3C Semantic Web Working Group.

## 14 Class C in BC2 compared with Class C in BC1

**14.1** The reasons for the radical nature of the revision of BC1 are considered in detail in the Introduction to BC2 (2).

**14.2** The general structure of C in BC1 is not unlike that in BC2:

| | |
|---|---|
| C | Chemistry |
| C1/C9 | . Common subdivisions |
| CA/CG | . General & physical chemistry |
| CA/CD | . . (Properties, processes, structures) |
| CE/CF | . . . Electrochemistry... Photochemistry... |
| CG | . . . Analytical chemistry |
| CH | . Mineralogy |
| | . . * Alternative (not recommended) is with geology at DN. |
| CI/CJ | . Inorganic chemistry & elements (non-metals) |
| CK/CN | . Inorganic chemistry & elements (metals) |
| CO/CR | . Organic chemistry |
| CS | . Biochemistry |
| | . . * Alternative to EI (which is preferred). |
| CT/CY | . Applied chemistry |

**14.3** The main differences from BC2 shown above are:

1. Inconsistent facet analysis, seen in the location of an operation (analysis) in the properties and processes facet.
2. The preferred location of Applied chemistry at CT/CY.
3. The prior division of the elements into Non-metals and Metals before the application of the periodic table.
4. The preferred location of mineralogy at CH.

**14.4** **Facets and arrays:** Within nearly all classes there is an absence of any clear distinctions between the facets and their arrays. For instance, in CA/CG there is frequent mixing up of processes and properties with structures; a major subclass of the Operations facet (Analysis) is mislocated and separated from the other operations and their agents at CA/CBB. In organic chemistry, when several different arrays are recognized (e.g., in CR Heterocycles) these are not consistently presented. For example, the array (By number of members in the ring) is clearly considered the primary array, but other arrays are misleadingly subordinated to rings of a specific size; for instance, the array Heteroatoms is subordinated to six-membered rings at CRH/J before the class for seven-membered rings appears.

**14.5** **Citation order:** Without a clear organization of terms into facets and arrays a consistent citation order is difficult to follow. No comprehensive statement is given and nearly all instances are implicit only, by virtue of subordination of one concept to another in the enumerated schedules. For instance, the Systematic Auxiliary Schedule for the subdivision of any element or compound implies the primacy of the Substances facet; there is repetitive subordination of techniques and equipment under different processes and operations.

**14.6** **Filing order:** Although no explicit principles are given, the enumeration reveals a roughly inverted schedule.

**14.7** **Notation:** The only provision for synthesis is that in the Systematic Auxiliary Schedule for the division of an element or compound. The relative brevity is partly due to the ordinal notation (of which Bliss was a pioneer), but even more is a result of the lack of specificity.

**14.8** **Vocabulary**: Some 900 separate concepts are recognized and the Auxiliary Schedule provides limited provision for an extension by synthesis to accommodate some compound concepts.

**14.81** This Class C in BC2 enormously increases the effective vocabulary. Some 3700 separate classes are enumerated. This is only the tip of the iceberg when the potential for synthesis is considered. Every concept in each facet is potentially combinable with every concept in each of the other facets. The resultant increase in the size of effective vocabulary is almost beyond measure.

## 15 Acknowledgements

**15.1** We are deeply indebted to Eric Coates, formerly Editor of the British Technology Index, and editor of the Broad System of Ordering (BSO) (24) for his invaluable and unstinting help throughout the production of this class, and this is acknowledged through his joint authorship. The Broad System of Ordering (BSO) Chemistry class was a most valuable ground plan for Class C, and although the latter deviates at a number of points from the BSO structure, the similarities between the two systems far outweigh their differences.

**15.2** We are also indebted to other friends and colleagues in the Classification Research Group for their patient discussions when the problems of schedule construction were taken to them. Dr Andrew Buxton (previously of University College London and Sussex University) also receives our sincere thanks for his painstaking analysis of the problems presented to him and his clarification of numerous chemical technicalities.

**15.3** The citation of papers by Brian Vickery and Robert Fugmann reflects the valuable help we received from their analyses of the problems faced. We also wish to acknowledge the help afforded in the matter of chemical vocabulary from the full edition of the UDC Class 54 Chemistry; a close working relationship has been established with the Editorial Board of UDC, with a mutually helpful exchange of on-going work.

**15.4** Finally, this volume is offered as a tribute to the memory of Jack Mills, who died during its preparation.

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# Summary outline of Class C: Chemistry

| | |
|---|---|
| C | Chemistry |
| C2 | . *Common subdivisions* |
| | . General operations & agents in chemistry |
| C36 | . . Practical chemistry, laboratory practice |
| C3U | . . . Equipment, apparatus, plant |
| C5X | . . . Reagents |
| C62 | . Investigative techniques in chemistry |
| C8E | . Preparative techniques |
| C8Y | . Synthesis |
| C9 | . Analysis, chemical analysis |
| | . . *Kinds of analysis by technique* |
| | . . . Microtechniques |
| | . . *Kinds of analysis by physical properties measured* |
| C9D | . . . Gravimetric analysis |
| V | . . . Volumetric analysis |
| C9M | . . . Spectrum analysis, spectroscopic analysis |
| C9Q | . . . Chromatography (analysis), adsorption analysis |
| | . . *Kinds of analysis by primary purpose* |
| C9Q V | . . . Qualitative analysis, detection |
| C9Q W | . . . Quantitative analysis, estimation |
| CA | . Physical chemistry, physics of chemistry |
| CAC | . . Chemical combination and structure |
| CAC F | . . . Chemical formulae |
| CAG | . . . Chemical bonds |
| CAO | . . . Molecular structure, structural chemistry |
| CAY | . . Reaction chemistry |
| CCA | . . . Catalysis |
| | . . . *Reactions by change in energy system* |
| CDU | . . . . Thermochemistry |
| CE | . . . . Electrochemistry |
| CER | . . . . Radiation chemistry |
| CES | . . . . . Photochemistry |
| | . . *Properties and processes in states of matter* |
| | . . . *Kinds of chemical systems* |
| CFL K/CFO | . . . . Mixtures, solutions, colloids |
| | . . . *Systems by pure state of matter* |
| CFS | . . . . Fluids |
| CFT | . . . . . Gases |
| CFU | . . . . . Liquids |
| CFV | . . . . Solids, solid state chemistry |
| CFW | . . . . . Crystalline state, crystal chemistry |
| CG | . Chemical species, chemical substances |
| CGE | . . Elements |
| | . . . *Kinds of elements by various characteristics* |
| CGE BPW | . . . . Isotopes |
| CQ | . . . . Polymorphous elements, allotropes |
| P | . . . Periodic table |
| CGF | . . . Individual elements |
| CGF X | . . Radicals |

# Summary outline of Class C: Chemistry

CGH . . Compounds
. . . *Kinds by various characteristics*
. . . . *Kinds by bonding characteristics*
CGH GCJ . . . . . Covalent compounds
GCL . . . . . Ionic compounds
. . . . *Kinds by variation in structure*
GCR . . . . . Isomers
. . . *Compounds by specific valency*
J . . . . Monovalent compounds
T . . . . Mixed valency compounds
Y . . . Acids, bases & salts together
CGI J . . . Complex compounds

CH . . . Inorganic compounds, inorganic chemistry
CJW . . . . Inorganic compounds by constituent elements
CJW Y . . . . . Group 1 elements
CKQ . . . . . Alkali metals
CKU . . . . . Group 2 elements, alkaline earth metals
CLD . . . . . P-block elements
CLE/CMY . . . . . Group 13-18 elements
CNA . . . . . D-block elements, transition metals
CNB . . . . . Group 3 elements, rare earths
CND/CNV . . . . . Group 4-12 elements
CNY . . . . . F-block compounds
CNY Q . . . . . Lanthanides
S . . . . . Actinides
VS . . . . . Transuranic elements

CO . . . Organic chemistry
COG . . . . Functional groups, organic radicals
. . . . *Organic compounds by constituent elements*
COI X . . . . . Hydrocarbons
COM Q . . . . . Organic compounds with heteroatoms
. . . . *Organic compounds by basic structures*
CP . . . . . Acyclic compounds, aliphatic compounds
CPR . . . . . Alicyclic compounds
CQ . . . . . Cyclic compounds
CQI X . . . . . Homocyclic compounds
CQY . . . . . Aromatic compounds
CR . . . . . Benzene
CS . . . . . Heterocyclic compounds
CTE . . . . Organic polymers
CTH . . . . Biologically significant organic compounds
CTJ . . . . . Lipids
CTQ . . . . . Carbohydrates
CUA . . . . . Alkaloids
CUD/CUF . . . . . Amino acids, peptides
CUH/L . . . . . Proteins, enzymes
CVW . . . . . Hormones
CWB . . . . . Vitamins
CWE . . . . . Natural pigments

CX . Applied chemistry, chemistry based technologies
. . * Alternative (not recommended) to Class U