

## Appendix 1: How to subdivide an element, compound or class of compounds

### How to subdivide an element, compound or class of compounds

- 1 The schedule for Class C is an inverted one (see Introduction Section 7). So in general, any class may be qualified (given subclasses) by adding to it all preceding classes, insofar as they are applicable. This is called retroactive synthesis. Exceptions to this are always noted in the schedule. The biggest exception occurs in the major class CJW/CNY Inorganic compounds by constituent elements, in which forward-building is also allowed.

The examples provided here do not introduce any new rules or provisions for subdivision but simply demonstrate the application of the existing retroactive synthesis. The examples are intended as a model for the way in which more complex topics are represented through synthesised classmarks, and how the schedule can be expanded to accommodate them.

### 2 Subdivision under an element (comprehensive works)

- 2.1 Provision is made (and individual elements enumerated) at CGF for completely comprehensive works dealing with the element per se and its inorganic and organic compounds together. Classes C2/CG are available for qualification by retroactive synthesis of the elements here, should the need arise, and an example is provided below. It is envisaged, however, that occasions where a document deals comprehensively with an element together with its inorganic and organic compounds, and also requires qualification by an earlier class will be very rare. Most of the literature on elements and their compounds falls under inorganic chemistry, and should be dealt with at CJW/CNY, as demonstrated at 3 below.

- 2.2 The order of subclasses under an element (where x stands for any element in CGF) is as follows:

- x Element x
- \* Classes x2/G are used for comprehensive works on the element, embracing information on the element per se and its inorganic and organic compounds in general.
  - \* For the element and its inorganic compounds, see CH/CNY; for its organic compounds, see COI Q/COP Y and CP/CW.

Comprehensive works on the element

- \* Add to x numbers and letters 2/F following C, e.g.,

(Operations)

Analysis

x9

x9M

x9QW

Spectrochemical analysis

Quantitative analysis

(Processes and properties)

xA

xABP

xAC

xACO

xAG

xAO

xAY

xES

Physical chemistry

Atomic properties

Chemical combination and structure

Stoichiometry

Bonding

Molecular structure, structural chemistry

Reaction chemistry

Photochemistry, photochemical properties and processes

- 2.3 Example of the subdivision of an element, using a specific element instead of an hypothetical x.

- 2.31 CGF LW Phosphorus chemistry  
(Comprehensive works on phosphorus)  
(Operations)  
Analysis  
CGF LW9 Spectrochemical analysis  
CGF LW9 M Quantitative analysis  
(Processes and properties)  
Physical chemistry of phosphorus  
CGF LWA Chemical combination and structure  
CGF LWA C Molecular structure, structural chemistry  
CGF LWA O Reaction chemistry  
CGF LWA Y Photochemistry of phosphorus, photochemical properties and processes  
CGF LWE S

## Appendix 1: How to subdivide an element, compound or class of compounds

### 3 Subdivision under an element/compound in inorganic chemistry

- 3.1 Inorganic chemistry provides the main location for the literature relating to the elements and their inorganic compounds. Organic compounds are dealt with under Organic chemistry, CP/CS. Documents in which an element, and its inorganic and organic compounds, are considered together are provided for at CGF, as described above.
- 3.2 As noted above, the schedule for Class C is an inverted one (see Introduction Section 7). So in general, any class may be qualified (given subclasses) by adding to it all preceding classes, insofar as they are applicable. The examples below demonstrate the application of this retroactive synthesis to effect the subdivision of any element, or compound, in inorganic chemistry. The Appendix does not introduce any new rules or procedures for classmark building beyond those normally used in the classification. The examples are intended as a model for the way in which more complex topics are represented through synthesised classmarks, and how the schedule can be expanded to accommodate them.
- 3.3 Exceptions to retroactive synthesis are always noted in the schedule. The biggest exception occurs in the major class CJW/CNY, Elements and groups of elements, in which forward-building is also allowed. This is to facilitate the bringing together (collocation) of an element and its compounds, even where constituent elements of some compounds are in later facets. For the convenience of the cataloguer/indexer all the major combinations of classes which involve forward building are pre-synthesised and included in the schedule.
- 3.4 The order of subclasses under an hypothetical Class x (where x stands for any element in CJW/CNY) is as follows:

x	Element x
	* Add to x numbers and letters 2/9,A/N following C; e.g.
x2	Common subdivisions (Operations and agents)
x9	Analysis (Processes and properties)
xA	Physical chemistry
xAY	Reaction chemistry
xF	(By change of state) (Types of x, compounds of x) (By preceding processes and properties)
xHFV	Solid state x (By valency)
xHJ	Monovalent x
xHY	Acids, bases and salts (together)
xIA	Acids of x
xIE	Salts of x
xIJ	Complex and coordination compounds of x
xJQ	(Compounds with other elements in general)
xJR	(Compounds with elements of particular Periods) * Compounds with elements of particular blocks or periodic groups are located by adding the appropriate classmark from CK/CNY; e.g., xLD Compounds with P-block elements.
xJT	(Compounds with metals) * General works only; compounds with a specific metal are located in the classes CK/CNY according to the citation order noted below. (Compounds by element(s) with which combined) * Citation order for classifying compounds follows the molecular formula so far as possible; otherwise it is retroactive. * When the molecular formula is followed, the addition of a second, third, etc element may have to be by building forward, not backward. This has been allowed for in the notation. * Filing order of elements is by groups of the periodic table.
xK	Compounds with hydrogen
xKJQ	Hydrides
xM	Compounds with oxygen
xMIA	Oxyacids
xNN	Compounds with Group 8 elements
xNO	Compounds with iron * If the molecular formula implies this order.

## Appendix 1: How to subdivide an element, compound or class of compounds

3.5 Example, using boron (CLF) instead of a hypothetical x:

CLF	Boron
CLF AY	Reaction chemistry
CLF HFW	Crystal forms
CLF HL	Divalent boron
CLF HV	Borides in general
CLF K	Compounds with hydrogen
	* Example of molecular formula rule allowing retroactive building of classmark (from CK Hydrogen).
CLF KHV	Boranes, boron hydrides
CLF M	Compounds with oxygen
	* Example of molecular formula rule requiring forward building of classmark (from CM Oxygen).
CLF MIA	Oxyacids of boron
CLF MIBN	Metaboric acid
	* Terminal N is valency (from HJN).

3.6 Subdivision of an individual compound is effected in exactly the same way, as the following example for Diborane (CLF KJH PP) shows (topics have been selected from a standard online search for articles on Diborane);

CLF KJH PP	Diborane, diboron hexahydride
CLF KJH PP8 E	Synthesis, preparative techniques
CLF KJH PPA G	Bonding
CLF KJH PPA IQ	Molecular orbitals
CLF KJH PPA J	Covalent bonds
CLF KJH PPA Y	Reactions, reaction chemistry
CLF KJH PPC HE	Nucleophilic reactions
CLF KJH PPD U	Thermochemistry
CLF KJH PPD VE	Endothermic reactions
CLF KJH PPF	Chemical systems, phases
CLF KJH PPF T	Gaseous phase
CLF KJH PPF TAY	Gaseous phase reactions

### 4 Subdivision under an organic compound

4.1 The note at 1 above applies here also. Because of the complexity of the structures in, and relationships between, organic compounds a very great number of them are enumerated in the schedule; it is not expected that those applying the classification will need, as a general rule, to synthesise classmarks for compounds. The following notes and comments are provided to indicate the analytical and structural principles that have been applied in developing the schedule, and to provide a model for those occasions when synthesis is required.

4.2 Subdivision is less simple than in the case of inorganic chemistry:

4.21 Elements are no longer the first-cited concept, being subordinated to the various categories of organic compounds at CP/CS. These categories (e.g. acyclic compounds, aromatic compounds, heterocycles) are further subdivided by:

4.211 i) functional groups: structural combinations of atoms or bonds that determine chemical properties and behaviour (e.g. esters, aldehydes, amides);

4.212 ii) organic radicals: parts of an organic molecule which relate to the parent hydrocarbon, and whose names are derived from them (e.g. methyl, propyl, butyl).

4.22 Names of functional groups and radicals between them provide the basis of systematic chemical nomenclature.

4.23 Because of the large number of functional groups to be accommodated at COI Q/COM P, division by elements only begins at COM R. From then on, the elements file in exactly the same order as in CJR/CN, but with the first letters changed as follows:

## Appendix 1: How to subdivide an element, compound or class of compounds

COM T/W is divided like CJT/W;  
COM X is divided like CK;  
CON is divided like CL;  
COO is divided like CM;  
COP is divided like CN.

Only in the case of hydrogen (COM X) and oxygen (COO) is the terminal letter different from that in CJ/CN.

- 4.24 A further difference is that the role of carbon, hydrogen and oxygen is primarily in defining the functional groups at COI Q/COM P, where they are cited after the other elements (not C, H or O) appearing as substituents in the basic structures.
- 4.25 The role of the elements other than C, H and O may also be regarded as defining functional groups and this is how they are characterized at COM R (Organic compounds by element, heteroatom functional groups). The term heteroatom is sometimes used to emphasize this role of the elements other than C, H or O. A cyclic compound containing one or more heteroatoms is referred to as a heterocyclic compound, or heterocycle.
- 4.26 The last important complication to be noted is that many of the basic structures have several arrays defining different classes of compounds. The general rule is that these arrays, representing different types of the basic structure concerned, are cited before specific elements. But a few exceptions occur; e.g. under CS Heterocycles the citation order is:

### Heterocycle

- i. (by size of ring)
- ii. (by element (the heteroatom) replacing a C in the ring)
- iii. (by saturation/aromaticity)
- iv. (by number of rings)

In this case, the element is cited before two arrays defining types of the basic structure of heterocycles.

- 4.27 It is important to note carefully the Add instructions applying to a given class. In order to help in this, a summary of the major ones governing CO/CW is given here (at 4.29). Additional ones may appear within a given class and these should always be noted carefully.
- 4.28 It is worth noting also that most Add instructions are given to confirm what retroactive classmark-building is to be allowed for; the first class to appear with a higher letter is the first enumerated subclass – i.e. one special to the class in question; e.g.

CQ       Cyclic compounds  
\* Add to CQ letters A/I following CO  
CQJ A     Cycloalkanes, cycloparaffins

- 4.29 Summary of organic chemistry and its major Add instructions:

CO       Organic chemistry  
\* Add to CO numbers and letters 2/F following C.  
COG      Functional groups, organic radicals  
(Kinds of functional groups)  
\* Add to COG G letters A/F following C, using the concepts as specifiers (species-makers)  
(Specific functional groups)  
\* Add to COG letters IX/PY following CO  
(Kinds of organic compounds)  
\* Add to COH letters GB/Y following CGH  
\* Add to CO letters IA/IN following CG  
COI Q     (Organic compounds by their constituent elements)  
COI X     Hydrocarbons  
COJ A     Alkanes...  
COL P     Alkynes...  
COL R     Oxygen with hydrocarbon compounds  
COM Q     Organic compounds with heteroatoms

## Appendix 1: How to subdivide an element, compound or class of compounds

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COM R	Elements, heteroatom functional groups * Add to CO letters MR/PY parallel with CJR/CNY (see note 4.23 above)
CP	(Organic compounds by basic structures) Acyclic, aliphatic compounds * Add to CP letters A/P following CO. (Types by homologous structure)
CPI Y	Saturated, alkanes...
CPJ Xs	Unsaturated
CPK A	Alkenes...
CPL A	Alkynes...
CQ	Cyclic compounds * Add to CQ letters A/MP following CO (By number of rings)
CQQ A	Monocyclic
CQQ B	Polycyclic (By mode of linkage)
CQQ CR	Separately bonded
CQQ CT	Condensed (By specific number of rings)
CQQ E	Bicyclic
CQQ I	Hexacyclic (By number of members in ring)
CQS	Three members
CQV	Six members
CQW B	Eight members (By special bond structures)
CQX	Alicyclic, non-aromatic
CQY	Aromatic
CQY V	Benzenoid compounds
CR	Benzene
CS	Heterocyclic compounds, heterocycles * Add letters A/I following CQ * Add letters IX/MP following CO (By number of rings in molecule) (By number of members in ring) * In heterocycles, this is the primary facet.
CTE	Organic polymers
CTH	Biologically significant organic compounds

### Radicals and functional groups

- 1 The term Radical is used with two distinct meanings:
- 1.1 For atoms or molecules with unpaired electrons, or an open shell configuration; these are highly reactive, and are alternatively called free radicals.
- 1.2 For collections of atoms which act as a unitary entity in reactions and largely characterize the chemical nature of the compounds in which they occur. Much the commonest form they take is that of functional groups in organic chemistry.
- 1.3 In the conventions for naming chemical compounds a distinction may be made between functional groups which determine chemical behaviour (e.g. amines, peroxides) and those which represent the length of the underlying hydrocarbon chain (e.g. methyl, propyl).
- 1.4 The general class, for works dealing with both these forms, is at CGF X.
- 1.5 Provision is made at CGG J/CGG N for specific radicals which function in both inorganic and organic chemistry (e.g., the hydroxide radical CGG MKJ) if a work deals with them in this respect.
- 2 Radicals in inorganic chemistry**
- 2.1 There is relatively little independent literature on specific free radicals compared with the large literature on specific functional groups in organic chemistry. Most of the literature deals with the compounds which contain the free radical as a constituent; these compounds are nearly always acids, bases or salts.
- 2.2 Provision is made at CGG J/CGG NY for works on specific inorganic radicals treated separately.
- 2.3 The general classmark for such a radical is derived from the main sequence of inorganic compounds as they occur under specific elements in CJ/CNY. Each classmark consists of the notations for its constituent elements combined in the order of the molecular formula, e.g.
- |         |                                  |
|---------|----------------------------------|
| CMQ M   | Compounds of sulphur with oxygen |
| CMQ MIE | Salts of sulphur with oxygen     |
| CMQ MIF | Specific salts                   |
- 2.4 If the compounded elements form more than one radical, they are distinguished by adding the valency number (from CGH J/CHG T); e.g.
- |           |                         |
|-----------|-------------------------|
| CMQ MIF P | Sulphites (tetravalent) |
| CMQ MIF S | Sulphates (hexavalent)  |
- 2.5 There is no separate listing of inorganic radicals as there is of functional groups in organic chemistry at COG. Synthesised classmarks for some of the most commonly occurring ones would be as follows:
- |             |                   |
|-------------|-------------------|
| CGG MKJ     | Hydroxide radical |
| CGG LML SHJ | Cyano radical     |
| CGG LMM IFP | Carbonate radical |
| CGG LVM IFJ | Nitrite radical   |
| CGG LVM IFL | Nitrate radical   |
| CGG LWM IFO | Phosphate radical |
| CGG MQM IFP | Sulphite radical  |
| CGG MQM IFS | Sulphate radical  |
- 3 Functional groups, organic radicals**
- 3.1 The general class for these is COG.
- 3.2 Classes of groups by various characteristics are given at COG G/COG GCWX; e.g.
- |            |                        |
|------------|------------------------|
| COG GAO XS | Difunctional groups    |
| COG GCW M  | Monosubstituted groups |
- 3.3 Specific groups by constituent elements. General works on these groups (i.e., dealing with their appearance in both aliphatic and cyclic compounds) go at COG IX/PY, where they are arranged in parallel with the compounds which are characterized by possession of the groups concerned.

## Appendix 2: Radicals and functional groups

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3.31 Whereas inorganic radicals are arranged primarily by their constituent elements taken in the order of their molecular formulae, organic groups are arranged by the basic structures (aliphatic, alkane, alkene, cyclic, etc.). Both alkyl radicals and functional groups may be seen to be derived by a process of hydrogen atom replacement; e.g. replacement of an H in Methane CH<sub>4</sub> gives the methyl radical CH<sub>3</sub>-; replacement of an H in Ethane C<sub>2</sub>H<sub>6</sub> gives the ethyl radical C<sub>2</sub>H<sub>5</sub>- and so on. Substitution of an H by a more complex functional group generates the classes of compounds characterized by them. By this token, the groups are sometimes referred to as substituents.

3.32 The general hierarchy of these derivations is roughly as follows:

COI X	Hydrocarbons
COJ A	Alkyl groups, alkanes... Alkenes... Alkynes...
COL R	Oxygen-containing functional groups
COL T	Alcohols... Ethers... Carbonyls...
COM R	Heteroatom functional groups (with elements not C,H or O)
CON S	Nitrogen... Diazo... Amines...

3.4 The detailed structure in the main sequence of organic compounds at CP/CS is achieved by a systematic subdivision of each large category of compounds (acyclic compounds, homocyclic compounds, heterocycles) by the functional groups. As a result there is consistency in the order of compounds under each of these broad groupings, and in the order of functional groups in Class CO. In order to accommodate additional detail, general categories of compounds may be qualified by more than one functional group, and/or by other characteristics such as valency. This process has been applied systematically, but the results are sometimes complex in nature; nevertheless they serve as a model for the indexer wherever there is a need for comparable expansion of schedule. Very occasionally, where there is no convenient principle of subdivision, subclasses may be enumerated, but this is normally only at a deep level of hierarchy.

4 To assist the ready locating of the commonest functional groups an A/Z list of those at COJ/COP is given below.

4.1 General classes for radicals and functional groups are provided by adding the notations at 4.2 to the base CO- (e.g. Alcohols COL T, Diolefins COK Q, Polyketones COM KR). Classmarks for organic compounds are similarly effected by adding the notations to the base number for the general class; e.g.

CP	Acyclic compounds
CPN S	Nitrogen acyclic compounds
CPN T	Amines
CQ	Cyclic compounds
CQJ A	Cycloalkanes
CQM K	Ketones

The great majority of such compounds are already pre-synthesised in the schedule, but further expansion can be achieved using the same principle.

Acetal	-MHL TW
Acetate	-MPN
Acetyl, ethanoyl, ethyl	-JC
Acetylene	-LC
Acyl, carbonyl	-MF
Alcohol	-LT
Alcoholate, alkoxide	-MXQ LT
Aldehyde	-MH
Aldoxime	-NTM H
Alkane group, alkyl	-JA
Alkanamide, amide, amido, carbamoyl, carbamyl	-NVR
Alkene, olefin	-KA
Alkoxide, alcoholate	-MXQ LT
Alkoxy	-LRJ A
Alkoxy carbonyl, carboxylate	-MFJ A
Alkyl, alkane	-JA

## Appendix 2: Radicals and functional groups

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Alkylthio, thioester	-OQM XMP
Alkyne	-LA
Allene, ketene	-MKX
Allyl, propenyl	-KD
Amide, alkanemide, amido, carbamoyl, carbamyl	-NVR
Amidine	-NVN SID
Amido, alkanemide, amide, carbamoyl, carbamyl	-NVR
Amine	-NT
Amino, primary amine	-NTR
Aryl	-LM
Azide	-NVN SNS
Azo	-NVN S
Azoxy	-NVN SOR
Benzenecarbonyl, benzoyl	-MFL N
Benzoyl, benzenecarbonyl	-MFL N
Benzyl, phenylmethyl	-LO
Butyl	-JE
Carbaldehyde, carboxaldehyde	-MMM H
Carbamoyl, alkanamide, amide, amido, carbamyl	-NVR
Carbamyl, alkanamide, amide, amido, carbamoyl	-NVR
Carbene	-JXH SS
Carbenium ion, carbonium ion	-JXH SS
Carbonium ion, carbenium ion	-JXH SS
Carbonyl, acyl	-MF
Carboxaldehyde, carbaldehyde	-MMM H
Carboxylic acid	-MM
Carboxylate, alkoxycarbonyl	-MFJ A
Carboxylic ester	-MPMM
Chloro	-OV
Cyano	-NVN MC
Decaalkyl	-JK
Diene, diolefin	-KQ
Dihydric alcohol, diol, glycol	-LW
Diketones	-MKS
Diol, dihydric alcohol, glycol	-LW
Diolefin, diene	-KQ
Disulphide	-OQM Q
Enamine	-NTK A
Enol, ketoenol	-MKU
Ethanoyl, acetyl, ethyl	-JC
Ethenyl, vinyl	-KC
Ethoxy	-LRJ C
Ethyl, acetyl, ethanoyl	-JC
Formyl, methanoyl, methyl	-JB
Glycol, dihydric alcohol, diol	-LW
Hydrazine, hydrazo	-NUV Q
Hydrazo, hydrazine	-NUV Q
Hydrazone	-NUV QS
Hydroximino, nitroso, oximide	-NVN SO
Hydroxy, hydroxyl	-LS
Hydroxyhydrazine	-NUV QLS
Imido	-NVS
Iodoso	-OXO
Isocyanate	-NVU
Isonitriles	-NVN MIF



## Appendix 2: Radicals and functional groups

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Ketene, allene	-MKX
Keto alcohol, ketol	-MKL T
Keto aldehyde	-MKM H
Keto enol	-MKU GS
Ketol, keto alcohol	-MKL T
Ketone	-MK
Ketoxine	-NTM K
Mercaptan, thiol	-OQM X
Methanoyl, formyl, methyl	-JB
Methoxy	-LRJ B
Methyl, formyl, methanoyl	-JB
Methylene	-KB
Nitramines	-NVT
Nitriles	-NVN MIF
Nitro	-NVN SOQ
Nitroso, hydroximino, oximido	-NVN SO
Nonaalkyl	-JJ
Octaalkyl	-JI
Olefin, alkene	-KA
Oximes, oximino	-NTL S
Oximido, hydroximino, nitroso	-NVN SO
Pentaalkyl	-JF
Peroxide	-MC
Phenyl	-LN
Phenylmethyl, benzyl	-LO
Polyalkene, polene	-KP
Polyene, polyalken	-KP
Polyketone	-MKR
Primary alcohol	-LTP
Primary amide	-NVR S
Primary amine, amino	-NTR
Propenyl, allyl	-KD
Propyl	-JD
Sulphone, sulphonyl, sulphoxide, sulphuryl	-OQO MQ
Sulphonyl, sulphone, sulphoxide, sulphuryl	-OQO MQ
Sulphoxide, sulphone, sulphonyl, sulphuryl	-OQO MQ
Sulphuryl, sulphone, sulphonyl, sulphoxide	-OQO MQ
Thioester, alkylthio	-OQM XMP
Thiol, mercaptan	-OQM X
Trihydric alcohol, triol	-LX
Triol, trihydric alcohol	-LX
Vinyl, ethenyl	-KC