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## **Categorisation of reference materials — Guidance on, and keywords used for RM categorisation**

*Catégorisation de matériaux de référence — Conseils sur, et mots-clés pour la catégorisation de matériaux de référence*

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## Foreword

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## Introduction

Reference materials are a major tool for assuring quality and reliability of results obtained in analysis and testing. Laboratories active in these fields often face problems in identifying reference materials which suit their needs. Although a large number of producers of (certified) reference materials exist, presentation of the product spectrum of each of these producers is largely heterogeneous and follows quite different principles which, in particular, causes the above problem.

Therefore, the aim of this TR was

- i) to study and compare existing classification and categorisation schemes for reference materials,
- ii) to develop RM features/characteristics upon which a harmonised and consistent categorisation scheme could be based, and
- iii) to investigate approaches for making the categorisation scheme adaptive to new RM needs and developments.



# Categorisation of reference materials — Guidance on, and keywords used for RM categorisation

## 1 Scope

The development of a harmonised categorisation scheme aims at facilitating a transparent and comparable presentation of reference materials by producers, and the identification of reference materials by users. The intended categorisation scheme should meet the needs of, and has to be developed with a specific view to, modern forms of information presentation and retrieval, i.e. internet-based catalogues and data bases

## 2 Existing categorisation schemes

Eight major categorisation schemes have been analysed, namely the scheme as proposed by ILAC, and schemes applied and used by LGC Promochem (for presentation of RM in 5 field-specific catalogues: clinical, environmental, food, inorganic, physical), COMAR, the VIRM database, FLUKA, IRMM, ERM, and the CCQM. Most of these schemes use different perspectives on RM for categorisation, and as a rule in a mixed (heterogeneous) form. In particular, this becomes obvious from the categorisation scheme used by the VIRM initiative which uses "discipline" and a "generic term" as categorisation criteria. The term list for "discipline" is not comprehensive, but homogeneous to a certain extent, while the term list for "generic" mixes up matrices and origins of (C)RM with properties and even uses and applications. Analyte and matrix are not categorised in the VIRM scheme. It should, however, be noted that VIRM uses more than one criterion for (C)RM description.

Main perspectives are the (certified, if applicable) reference property carried by the material, the field of application, and the analyte and/or matrix. The extent to which the different perspectives are mixed is different for different schemes, but a certain heterogeneity is always present. LGC Promochem simply sub-divides the whole set of available RM and assigns the sub-groups to five different catalogues with the aim to assure that the within-catalogue categorisation scheme does not become too heterogeneous and matches terminologies established within the different fields of application. Although the CCQM scheme is the most homogeneous of all schemes considered, the degree of detailing is not very high. A scheme designed to facilitate the identification of reference materials by users should therefore be designed by integration of the various reasonable approaches of the above (and other, if available) schemes.

For pharmaceuticals, the USP model for drug characterisation was investigated with a clear view to therapeutic categorisation which is mainly governed by defining (groups of) active agents with specific potency and, consequently, specific uses and applications.

## 3 The harmonised scheme

### 3.1 Basic principles

Given the results of the above preliminary study, the following basic ideas can be developed for a harmonised categorisation scheme.

Depending on the intended purpose of a reference material, the valuable property (i.e. the one a customer pays for and which normally also distinguishes this specific material from the rest) may be of different kinds. There are RM carrying an obviously material-dependent property, however the material itself is of minor or no interest to the user since the user is interested only in this specific property. This is the reason why "single" categorisation schemes are normally heterogeneous.

**EXAMPLE** An oil may e.g. be produced to carry a certain value of viscosity, and customers will not (or at least only to a minor extent) be interested in knowing whether the oil is mineral or synthetic. On the other hand, for a transformer oil developed for residue analysis (e.g. PCBs), viscosity may be of minor or no interest to the user since the analytical method of choice normally includes a matrix separation.

Heterogeneous categorisation schemes often create problems in assigning the appropriate category to a specific material, especially when more than one apply. On the other hand, the degree of detailed description may be extremely different for the different categories of the scheme.

**EXAMPLE** Compare e.g. a group named "low alloy steels" with a group called "life science applications". The latter is clearly in disadvantage.

It cannot be the intention of the categorisation scheme to assign a unique keyword sequence to each and every RM, existing or intended to be produced. This makes such a scheme different from e.g. the unique identification of a substance by a CAS number. The only intention is to provide a descriptive tool allowing the creation of sufficiently large (for representativeness) and sufficiently fine-tuned groups of resembling RM. Group sizes may significantly vary from group to group depending on the total number of RM available on the market for the specific purpose, and the (economic and scientific) importance of this share.

Given this, an ideal categorisation scheme should be

- i) "as distinctive as possible" (i.e. a possibly more detailed description for distinction)
- ii) "as appropriate as necessary" (i.e. good enough for separating between different purposes/uses, but not unique).

These goals cannot be achieved within the framework of one single, stiff categorisation scheme even if one allows the scheme to be (extremely) heterogeneous.

### 3.2 Layout

Reference materials should therefore be categorised in a more descriptive, flexible approach. This approach describes the material according to the three criteria identified earlier, namely

(certified) reference property - (field of) application - analyte and matrix.

For each of the three criteria, lists of keywords (i.e. groups and subgroups) are given in Annex A. Criteria/descriptions of a specific RM (consider the oil carrying a value for viscosity) which do not apply may be left out in the description. This should appropriately be indicated in the presentation.

The keywords of the categorisation schemes used or proposed by ILAC, LGC Promochem (5 catalogues), COMAR, FLUKA, IRMM, ERM, and the CCQM (as studied under clause 2) have been split off according to the three criteria (or perspectives) to look at an RM. From the collation of keywords from all schemes, the list as presented in Annex A was generated. This "symbiosis" list was created with the intention of either including a specific key word from a particular categorisation scheme or making sure that a coarse category (e.g. "High-purity chemicals") could be described by a combination of criteria from the symbiosis list.

RM carrying two or more different reference properties cannot be described by a single category sequence.

**EXAMPLE** Consider e.g. a silicon nitride certified for trace element content and phase composition.

In such situations, several keyword sequences (according to the number of reference properties carried by the material) can be attributed. From the point of view of information retrieval, this will ensure that the material can be found and compared with competitive materials for all purposes/usages for which it is intended.

### 3.3 Recommendations

The keywords as listed in Annex A are intended for structuring, in a harmonised way, the presentation of any particular set of reference materials offered to the customer. It may be applied to any presentation form but mainly to databases and catalogues, both electronic and printed.

It must be pointed out that the scheme as proposed in Annex A does not affect the producer's internal scheme of attributing serial or otherwise structured numbers to particular materials. It is for external presentation, search and retrieval purposes only.

The scheme could be understood as an offer made to RM producers. Depending on the intention of the producer and the kind of the material, producers may select the degree of detail they implement in the keyword sequence. Certainly the recommendation for a "as good as possible" description using the available category keywords can be given, but it is up to the producer to decide whether or not a particular keyword applies and should be included in the presentation.

Producers should therefore decide about the number of criteria they wish to apply for structuring their production profile presentations. It is in no way mandatory to use all ordering criteria. In principle, any set of reference materials should be categorised

- i) with a satisfactory degree of distinction between the different materials but
- ii) without the intention to make all categories unambiguous.

The above principle equally applies to the number of criteria used, and the keyword sub-level attributed to a particular reference material.

**EXAMPLE** Depending on the position of a particular producer of food reference material in the market, it may be sufficient to use e.g. the category "beverages" if it is known that the producer specialises in e.g. non-alcoholic beverages. If this is not the case, a lower sub-level (e.g. "alcoholic and low alcohol beverages") should be chosen in order to distinguish these products from others.

It is, however, not recommended to mix up categories originating from, and belonging to, different aspects/criteria of categorisation.

## 4 Reporting attributed keywords

For electronic search and data retrieval, catalogue search using the descriptive keywords in the three categories as given is recommended. Producers and distributors of reference materials operating data retrieval systems which are publicly accessible and/or provide product lists or catalogues should analyse the ways (i.e. perspectives) used by customers to seek information on the availability of a specific reference material meeting customers' needs. Experience shows that almost all three main perspectives (certified property, field of application, and analyte/matrix combination) are used by customers potentially interested in reference materials.

Providers of electronic or written data collections on reference materials (producers, distributors, consultants, etc.) should therefore

- i) categorise each material available as fully as possible according to the keywords given in Annex A
- ii) indicate, for each material, the above defined descriptive keywords in an appropriate form. Possible forms are e.g. sub-headers on printed material specifications and/or in printed catalogues, and specific search fields in electronic data collections.
- iii) provide search tools for the above defined keywords (catalogue search).

**NOTE** It is not always feasible, in some cases even senseless, to attribute keywords for all three main perspectives/criteria to any particular reference material. Reference materials for e.g. dimensional properties do not contain "analytes",

and the material they are made of is normally of minor importance (at least for the user). In those cases, the corresponding categorisation field should be left blank or filled in with "n/a" (see also clause 3).

Thus, a complete categorisation may look like

```
reference property:  nutritional properties
application:        food analysis
analyte:           ethanol and alcohol congeners
matrix:            alcoholic and low alcohol beverages
```

and describes the property as nutritional, the field of application as food analysis, the analyte as ethanol and alcohol congeners, and the matrix as alcoholic and low alcohol beverages. There may be doubts whether an alcoholic content is actually a "nutritional" property. For being on the safe side, the first descriptor could be replaced by "food properties".

## 5 Category keyword coding

Providers of electronic or written data collections on reference materials might wish to convert the keyword sequences attributed to reference materials into a machine-readable code. Appropriate coding schemes for the generation of a compact descriptive identifier which can be used for all information retrieval purposes may be developed in different ways. A simple coding scheme could be based upon the following principles: Three digits for each of the criteria "Reference value" and "Application" are reserved, although not all of them may be occupied depending on the sub-group level used for categorisation. "Analyte" and "Matrix" are described by four digits each, combined giving an (up to) 8-digit code for this criterion. The first digit for each criterion is alpha-numeric, the others are numbers. Codes generated from these rules are not descriptive for the key word although there are some correlations, especially for the matrix criterion. As a code for "not applicable" a numerical zero may be used in the first digit of the corresponding criterion, distinguishing it clearly from the letters in case the criterion is applicable.

NOTE It should be pointed out that this "machine-readable" code generated for electronic search and retrieval purposes is not intended to be printed in the documentation accompanying the reference material, as e.g. passport, certificate, label or other (although this option is not excluded).

EXAMPLE The following examples of how the descriptors of the proposed scheme could be applied are taken from different CRM producers and refer to different materials with different fields of application.

Material: ERM BA005 Lager 5% ABV (alcohol by volume) (5.07 +/- 0.03 %ABV). As shown under item point 4, the complete categorisation would be

```
reference property:  nutritional properties
application:        food analysis
analyte:           ethanol and alcohol congeners
matrix:            alcoholic and low alcohol beverages
```

Material: NIST SRM 3145a - Rubidium Standard Solution. The categorisation would be

```
reference property:  trace component content
application:        single element standards for ICP
analyte:           alkali metals
matrix:            solvents
```

## Annex A

### List of keywords for RM categorisation

#### A.1 Keywords according to criterion I: (Certified) reference property

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
biological properties	biological activity	
	GMO content	
	enzyme activity	
	protein interaction	
cell properties	object number	
	multiplication/decay rate	
chemical composition	blanks	
	extractable element content	
	isotope abundance ratio	
	major components	
	mixtures	
	purity	
	stoichiometry	
	species content	
	trace component content	
chemical properties	atomic weight	
	molecular weight	
	catalytic activity	
	chain length	
	identity	
	polarity	
	sequence	
fire resistance properties	flammability	
	smoke density	
food properties	blanks	
	fatty acid profile	
	nutritional properties	
	proximate analysis	
	triglyceride composition	

## ISO/PDTR

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
physical properties		moisture
	age	
	dimensional	length volume roundness
	electrical	conductivity dielectric strength resistivity
	magnetic	magnetic susceptibility
	mechanical	
	optical	colour density optical rotation refractive index reflectance spectral absorbance spectral emission spectra parameters
	physicochemical properties	density electrophoretic mobility pH surface tension viscosity
	radioactivity	
	structural properties	crystallographic structure morphological properties phase composition single crystal cell parameters
thermodynamic properties	boiling point Curie point enthalpy and heat capacity melting, freezing and triple points	

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
		temperature fixed point thermal conductivity thermal expansion thermal resistance vapour pressure
technical properties		
	abrasive wear rate scratch resistance corrosion rate creep rate elasticity flash point hardness impact toughness fracture toughness tensile strength	
humidity		
properties of films and surfaces		I
	depth profiling ion beam sputtering nominal thickness particle backscattering x-ray fluorescence surface finish surface roughness	
sizing		
	particle number particle distribution particle flow particle size porosity surface area	
miscellaneous		

## A.2 Keywords according to criterion II: (Field of) application

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
age determination buffer systems		
calibration		
	electrode calibration spectrochemical materials	

## ISO/PDTR

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
	spectrochemical solutions	single element solutions for ICP single element solutions for AAS multielement solutions for ICP multielement solutions for AAS
cell biology		
clinical/medical applications	bacteriology and mycology clinical chemistry general medicine haematology and cytology immunology molecular biology	DNA profiling DNA sequencing
	parasitology tissue pathology virology other clinical/medical	
cosmetic industry electrophoresis		
field-specific applications	elemental analysis environmental analysis fluorescence analysis food analysis geochemical analysis geophysical analysis metal analysis radiation dosimetry speciation thermal analysis	
fire research forensic applications		
identity and authenticity test	fibre identification substance identification	
method-specific applications	chromatography	

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
		GC ion chromatography LC
	dosimetry microscopy spectroscopy titration x-ray diffraction	
non-destructive testing		
	dye penetration magnetic particle inspection	
pharmacopoeial standards miscellaneous		

### A.3 Keywords according to criterion IIIa: Analyte description

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
chemical elements		
	alkali metals alkali earth metals halogens metalloids noble gases non-metals other metals rare earth metals transition metals	
electrolytes ethanol and alcohol congeners		
ions		
	anions cations isotopically labelled compounds	
isotopes		
	stable isotopes radioactive isotopes radiogenic isotopes	
metal-containing compounds		
	minerals metallo-organic compounds	
organic compounds		

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
	additives	antioxidants emulsifiers plasticisers vulcanising agents fillers
	amino acids carbohydrates chiral compounds copolymers creatinine DNA, RNA drugs of abuse enzymes erythrocyte protoporphyrine ethylglucuronide hormones lipids mycotoxins peptides pesticides, herbicides, acaricides, and metabolites polymers	
	priority pollutants	AOX BTEX heavy metals and metal species organo tin compounds PAH polyhalogenated compounds TPH
	proteins steroids toxins	animal origin plant origin other biological origin
	therapeutic drugs	analgesics anesthetics antibacterials anticonvulsants antidementia Agents antidepressants antidotes, deterrents, and toxicologic Agents antiemetics antifungals antigout agents anti-inflammatories

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
		antimigraine Agents antimyasthenic Agents antimycobacterials antineoplastics antiparasitics antiparkinson Agents antipsychotics antivirals anxiolytics bipolar Agents blood Glucose Regulators blood products blood modifiers blood volume expanders cardiovascular agents central nervous system agents dental and oral agents dermatological agents enzyme replacements/modifiers gastrointestinal agents genitourinary agents hormonal agents, stimulant/replacement/modifying hormonal agents, suppressant immunological agents inflammatory bowel disease agents ophthalmic agents otic agents respiratory tract agents sedatives/hypnotics skeletal muscle relaxants therapeutic nutrients/minerals/electrolytes
	veterinary drugs vitamins VOC	
respirable silica radiopharmaceuticals miscellaneous		

#### A.4 Keywords according to criterion IIIb: Matrix description

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
agricultural chemicals and fertilisers animal tissues ashes, dusts biological reference cultures bio-stabilisation products carbides catalysts		

## ISO/PDTR

cements, clays and related products

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
	ceramics, glasses and refractory oxides	
	dyes	
	explosives, primers, and degradation products	
	flammable liquids and residues thereof	
food		
	additives	
	dyes	
	preservatives, antioxidants	
	spices	
	beverages	
		alcoholic and low alcohol beverages
		non-alcoholic beverages
	fruits and vegetables	
		fruits
		cereals and crops
	dairy products	
	fats	
		animal oils and fats
		vegetable oils and fats
	fish	
		sea and freshwater fish
		molluscs
		plankton
	meat	
	processed food	
fibres		
	asbestos fibres	
	natural fibres	
	synthetic fibres	
filters and filter media		
genetically modified objects		
glasses		
	automotive	
	bottle	

main group	sub-group 1 <sup>st</sup> level	sub-group 2 <sup>nd</sup> level
	spectacle window	
human body fluids	blood serum saliva urine	
human body tissues	bone hair teeth	
industrial acids and bases		
metals	cast irons high purity metals	
	non-ferrous metals and alloys	brasses bearing alloys Al, Mg, Si and alloys light (Li, Be), alkali and alkaline-earth metals Cu, Zn, Pb, Sn, Bi and alloys Ni, Co, Cr and alloys Ti, V, Zr and alloys
	precious metals and alloys rare earth metals refractory metals and alloys	
	steels	by-products carbon steels cast steels high alloy steels low alloy steels special alloys unalloyed steels
minerals		
mineral processing materials	furnace matte converter matte	

## ISO/PDTR

concentrate  
mill feed  
tails

### main group

### sub-group 1<sup>st</sup> level

### sub-group 2<sup>nd</sup> level

noxious substances  
ores and rocks  
oxides, salts

petroleum products

heat exchange fluids  
liquid fuels  
oils and lubricants  
solid fuels

paints and varnishes

architectural  
automotive

particulate materials  
plastics and rubbers

plants

aquatic plants  
grasses and crops  
trees and bushes  
other

polymers

sediments

freshwater sediments  
marine sediments

sludges  
soils  
solvents

wood

wood products

waste

water

potable water  
fresh water  
sea water  
industrial waste water  
sewage

miscellaneous