

ANALYTICAL CHARACTERISATION OF UVCBs FOR REACH

WHITE PAPER

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the **REACH** CENTRE

It is the responsibility of every legal entity making a registration under REACH to provide analytical characterisation data that demonstrate the identity and composition of the substances they manufacture or import.

INTRODUCTION

Substances of **U**nknown or **V**ariable composition, **C**omplex reaction products or **B**iological materials (UVCB) are substances in which:

- The number of constituents is relatively large and/or
- The composition is, to a significant extent, unknown and/or
- The variability of composition is relatively large or poorly predictable

By their very nature, UVCB substances can present a difficult analytical challenge and their characterization demands a somewhat different approach to that used for well-defined (mono- and multi-constituent) substances. Typical examples of UVCBs include petroleum products, plant-derived essential oils and complex inorganic species such as minerals.

Formal substance identification involves several elements:

- The main identifiers including the name, source and relevant steps of the production process
- Analytical data appropriate to the substance in question
- Other relevant parameters such as boiling range or optical activity

Substance identity is frequently defined by the commercial sector within which each UVCB is produced and marketed. Formal quality standards are usually set that must be fulfilled in order for a substance to be sold for a given application. This usually includes at least some analytical information that could be used as a point of reference.

DESIGNING AN APPROPRIATE ANALYTICAL STRATEGY FOR REACH REGISTRATION OR INQUIRY

GENERAL GUIDANCE

Any analytical strategy that is developed should take into account the following requirements:

- The chemical composition and identity of the constituents should be given *as far as known*. This information can be provided in a generic way if appropriate, e.g. the carbon chain-length range.
- Unknown constituents should be identified using a generic description of their chemical nature if this is possible.
- Typical concentrations and concentration ranges need to be given
- All constituents present at a concentration of $\geq 10\%$ should be specified by an English IUPAC name and a CAS number.
- All constituents of relevance to PBT assessment or classification must be identified by at least an English IUPAC name and a CAS number, irrespective of their concentration.

IN PRACTICE

- Both spectroscopic and chromatographic data should be provided where this is scientifically meaningful and practically possible. Spectral data are used to define the *identity* of the substance whilst chromatography defines its overall *composition*.
- Spectra and chromatograms of UVCBs are generally complex and tend to take the form of 'fingerprints'. Consequently, interpretation may rely on comparison with analytical laboratory standards and published reference material. At least some of the individual components can usually be identified.
- In addition to spectroscopy and chromatography, the determination of other physical parameters may be appropriate. Depending on the nature of the substance, these could include optical rotation, boiling or melting points/ranges, crystal size and shape and enzyme activity.
- Scientific justification for tests not deemed to be appropriate must be provided. This is typically limited to the principal spectroscopic and chromatographic techniques.

SUITABLE ANALYTICAL TECHNIQUES

ORGANIC UVCBS

- Unless technical reasons dictate otherwise, the minimum spectroscopic data required for substance identification should include:
 - NMR (Given the complexity of UVCBs, both ^1H and ^{13}C NMR are likely to be appropriate)
 - FT-IR
 - UV-visible(Mass spectrometry of UVCBs is best undertaken as part of the chromatographic analysis)
- At least one type of chromatography should be included to demonstrate the overall composition of the substance. The specific technique will depend on various physical parameters including volatility, solubility and stability. In some instances, it may be necessary to use more than one type of chromatography. For example:
 - GC-MS is particularly useful technique for UVCBs containing volatile components.
 - HPLC-MS is more appropriate for soluble, larger molecules with lower volatility.

INORGANIC UVCBS

- In this case, substance identity should be demonstrated using at least the following techniques (unless technical reasons dictate otherwise):
 - XRD
 - FT-IR spectroscopy
 - UV-visible spectroscopy
 - NMR spectroscopy (where specific elements are present in the substance)
- The overall composition of the substance should be demonstrated by at least one of the following:
 - XRF or ICP-OES/ICP-MS or AAS or SEM-EDX (for elemental composition)
 - Ion chromatography (for determination of specific ionic components)
- Other analyses such as acid/base titration may also be appropriate in certain cases.

SUPPORTING DOCUMENTATION

Results should be fully interpreted and all experimental work (and reference materials used) comprehensively documented such that a competent person might be able to repeat the work.

GLOSSARY OF TERMS	
AAS	Atomic absorption spectroscopy
FT-IR	Fourier Transform infrared spectroscopy
GC-MS	Gas chromatography with mass spectrometry
HPLC-MS	High performance liquid chromatography with mass spectrometry
ICP-MS	Inductively coupled plasma with mass spectrometry
ICP-OES	Inductively coupled plasma with optical emission spectroscopy
NMR	Nuclear magnetic resonance
SEM-EDX	Scanning electron microscopy with energy dispersive X-rays
UV-vis	UV-visible spectroscopy
XRD	X-Ray diffraction
XRF	X-Ray fluorescence

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