

ANALYTICAL CHARACTERISATION OF WELL DEFINED SUBSTANCES FOR REACH

PART TWO: INORGANIC SUBSTANCES

WHITE PAPER

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November 2011

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

Mono- and multi-constituent inorganic substances are regarded as having a well-defined composition.

- A mono-constituent substance is *"a substance, defined by its quantitative composition, in which the main constituent is present to at least 80 % (w/w)"*.
- A multi-constituent substance is *"a substance, defined by its quantitative composition, in which more than one main constituent is present in a concentration $\geq 10\%$ (w/w) and $< 80\%$ (w/w)"*.

Arguably, the characterisation of inorganic substances, whether mono- or multi-constituent, relies to a greater extent on non-spectroscopic analytical techniques than does the characterisation of organic substances. Elemental analysis, determination of the ionic content, degree of hydration and crystal morphology are often particularly important. Regardless of whatever suite of tests is selected, the combined results obtained must demonstrate unequivocally the identity and purity profile of the substance in question.

DESIGNING AN APPROPRIATE ANALYTICAL STRATEGY FOR REACH REGISTRATION

GENERAL GUIDANCE

- The analytical strategy must be able to identify and quantify all the major components in the substance.
- Impurities present at a concentration of $\geq 1\%$ w/w should be identified and identified. They should then be specified by the following:
 - Chemical name
 - EC and/or CAS number
 - Molecular formula
- Any impurities of relevance for classification and/or PBT assessment should be specified as above, regardless of their concentration.
- The sum of the main constituents, impurities and any additives included to preserve the stability of the substance must be 100%

IN PRACTICE

- If the substance is crystalline, its identity should be demonstrated by XRD.
- Supporting evidence should be provided using the following techniques (unless technical reasons dictate otherwise):
 - FT-IR spectroscopy
 - UV-visible spectroscopy
 - NMR spectroscopy
- 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
 - Ion chromatography
- Other analyses, such as titrations or electron microscopy, may also be appropriate in certain cases.
- Scientific justification must be provided for tests not deemed to be appropriate. This is typically limited to the principal spectroscopic and chromatographic techniques listed in Annex VI of REACH (Section 2: *Identification of the Substance*).

SUPPORTING DOCUMENTATION

Results should be fully interpreted and all experimental details (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
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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