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Gas analysis — Purity analysis and the treatment of purity data

Analyse des gaz — Analyse de pureté et traitement des données de pureté

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Foreword

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For an explanation on the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the WTO principles in the Technical Barriers to Trade (TBT) see the following URL: Foreword - Supplementary information

The committee responsible for this document is ISO/TC 158, *Analysis of gases.*

Introduction

The use of purity data in the calculation of the composition of calibration gas mixtures is an essential element in establishing metrological traceability of the certified gas composition. Purity analysis is usually challenging, as normally, trace levels of various components need to be determined in a matrix for which limited or no measurement standards are readily available.

In many practical situations, purity data in some form are available. For the preparation of calibration gas mixtures, it is important that this information is interpreted in a consistent fashion and taken into account in the calculation of the composition of the mixture.

Gas analysis — Purity analysis and the treatment of purity data

1 Scope

This International Standard sets requirements for the purity analysis of materials used in the preparation of calibration gas mixtures and the use of these data in calculating the composition of the mixture thus prepared.

2 Normative references

The following documents, in whole or in part, are normatively referenced in this document and are indispensable for its application. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 6143, *Gas analysis — Comparison methods for determining and checking the composition of calibration gas mixtures*

ISO 7504, *Gas analysis — Vocabulary*

ISO 14912, *Gas analysis — Conversion of gas mixture composition data*

ISO/IEC Guide 98-3, *Uncertainty of measurement — Part 3: Guide to the expression of uncertainty in measurement (GUM:1995)*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 7504 apply.

4 Symbols

In this International Standard, the following symbols are used:

i running index over the components in a mixture

j index of the parent gas

k index of a specific component in a mixture

L_{ij} limit of detection of component i in parent gas j

u standard uncertainty (of the quantity between brackets)

w_{ij} mass fraction of component i in parent gas j

x_{ij} amount–of–substance fraction of component i in parent gas j

ϕ_{ij} volume fraction of component i in parent gas j

5 Principles

5.1 General

The determination of the impurities contained in each material (gas or liquid) used in the preparation has an impact on the uncertainty associated with the content of the component.

Assess and list all of the impurities that might be present in the material. These can be identified by different means, including

— open literature,

— information provided with the material,

— previous experience of using the same or similar materials, and

— knowledge of the process used to produce the material.

In order to decide the extent of purity analysis required, it is necessary to specify which of the potential impurities are 'critical' and which are 'significant' to the final composition of the mixture.

5.2 Assessment of critical and significant impurities

5.2.1 Critical impurities

A critical impurity is an impurity that meets one or more of the following criteria:

— an impurity in the parent gas or liquid of a mixture that is also present as a minor component in the same mixture at low concentrations;

EXAMPLE If preparing a low-concentration oxygen in nitrogen mixture, oxygen might also be present as an impurity in the nitrogen.

— an impurity that has the potential to influence the result of an analytical verification of the mixture composition;

EXAMPLE The presence of argon in nitrogen or oxygen will influence the analytical verification of the oxygen content when using gas chromatography with a non-selective detector.

— an impurity in a parent gas or liquid of a multi-component mixture that is also present as a minor component in the same mixture;

EXAMPLE For natural gas mixtures, *i*-pentane is often found as an impurity in *n*-pentane and *neo*-pentane, as well as being added as a minor component in its own right.

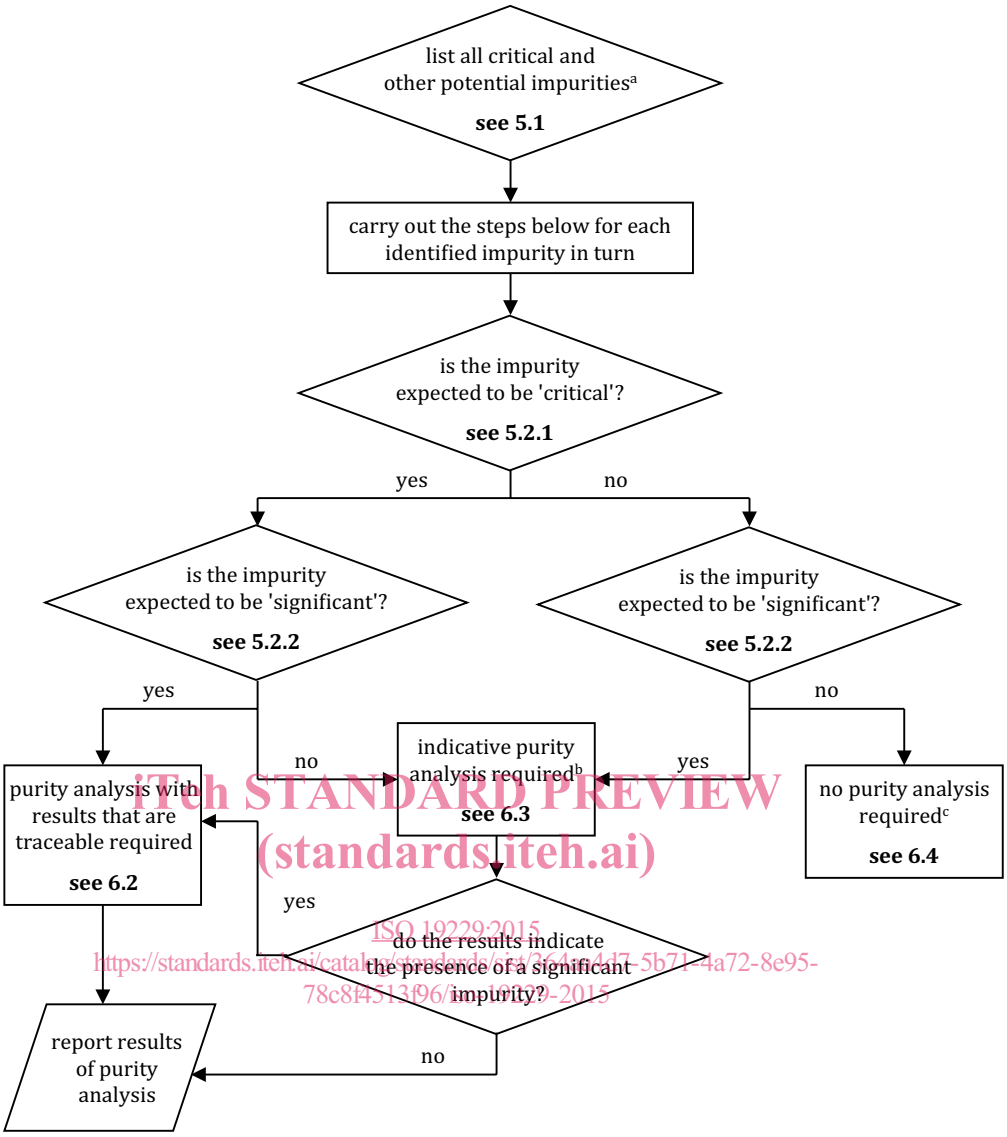
— an impurity that might be reactive with respect to any other component in the mixture.

EXAMPLE If preparing a mixture of nitric oxide in nitrogen, any oxygen present as an impurity in the nitrogen might react with the nitric oxide to form nitrogen dioxide.

5.2.2 Significant impurities

A significant impurity is an impurity that is predicted to contribute more than 10 % to the target uncertainty of the content of any of the components in the calibration gas mixture. The application of this criterion requires knowledge of the preparation method used (e.g. gravimetric, volumetric, static, or dynamic) and the uncertainties associated with the various steps involved.

The above described steps are summarized as a flowchart in Figure 1. The use of the flowchart is explained in the following subclauses.



a If an unpredicted or unknown impurity is identified during the course of a purity analysis, return to the start of the flowchart.

b If preferred, a purity analysis with results that are traceable can be carried out instead of an indicative purity analysis.

c If preferred, a traceable or indicative purity analysis can be carried out.

Figure 1 — Purity analysis flowchart

6 Analysis of impurities

6.1 General

The extent of purity analysis required shall be determined by the outcome of the flowchart in Figure 1. Each of these levels is discussed in 6.2 to 6.4.