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Surface chemical analysis — Secondary ion mass spectrometry — Calibration of the mass scale for a time-of-flight secondary ion mass spectrometer

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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT) see www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 6, *Secondary ion mass spectrometry*.

This second edition cancels and replaces the first edition (ISO 13084:2011), which has been technically revised.

The main changes to the previous edition are as follows:

— addition of Annex B (informative), *Internal addition method*.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

Secondary ion mass spectrometry (SIMS) is a powerful technique for the analysis of organic and molecular surfaces. Over the last decade, instrumentation has improved significantly so that modern instruments now have very high repeatability and constancy[2]. An increasing requirement is for the identification of the chemical composition of complex molecules from accurate measurements of the mass of the secondary ions. The relative mass accuracy to do this and to distinguish between molecules that contain different chemical constituents, but are of the same nominal mass (rounded to the nearest integer mass), is thus an important parameter. A relative mass accuracy of better than 10 ppm is required to distinguish between C_2H_4 (28,031 30 u) and Si (27,976 92 u) in a parent ion with total mass up to 1 000 u, and between CH_2 (14,015 65 u) and N (14,003 07 u) in parent ions with total mass up to 300 u. However, in a recent interlaboratory study[3], the average fractional mass accuracy was found to be 150 ppm. This is significantly worse than is required for unambiguous identification of ions. A detailed study[4] shows that the key factors degrading the accuracy include the large kinetic energy distribution of secondary ions, non-optimized instrument parameters and extrapolation of the mass scale calibration.

This document describes a simple method, using locally sourced material, to optimize the instrumental parameters, as well as a procedure to ensure that accurate calibration of the mass scale is achieved within a selectable uncertainty.

Surface chemical analysis — Secondary ion mass spectrometry — Calibration of the mass scale for a time-of-flight secondary ion mass spectrometer

1 Scope

This document specifies a method to optimize the mass calibration accuracy in time-of-flight secondary ion mass spectrometry (SIMS) instruments used for general analytical purposes. It is only applicable to time-of-flight instruments but is not restricted to any particular instrument design. Guidance is provided for some of the instrumental parameters that can be optimized using this procedure and the types of generic peaks suitable to calibrate the mass scale for optimum mass accuracy.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

No terms and definitions are listed in this document.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at http://www.electropedia.org/

4 Symbols and abbreviated terms

4.1 Symbols

m	mass of interest
m_1	calibration mass 1
m_2	calibration mass 2
M	mass (u)
M_0	the peak centre (u)
ΔM	mass accuracy (u)
M_P	measured peak mass (u)
M_T	true mass (u)
$U(m)$	mass uncertainty for a mass, m, arising from calibration
U_1	uncertainty in the accurate mass measurement of m_1
U_2	uncertainty in the accurate mass measurement of m_2