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

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Foreword

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This document was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 6, *Mass spectrometries*.

This third edition cancels and replaces the second edition (ISO 13084:2018), which has been technically revised.

The main changes are as follows:

— addition of informative Annex B.

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]. A growing need 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, which is significantly worse than the accuracy needed 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 — Mass spectrometries — 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. This document is only applicable to time-of-flight instruments but is not restricted to any particular instrument design. This document gives guidance 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 terminology databases for use in standardization at the following addresses:

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

— IEC Electropedia: available at https://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	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