



Standard Guide for Interpretation of Mass Spectral Data Acquired with Time-of-Flight Secondary Ion Mass Spectroscopy¹

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1. Scope

1.1 This guide provides time-of-flight secondary ion mass spectrometry (ToF-SIMS) users with a method for forms of interpretation of mass spectral data. This guide is applicable to most ToF-SIMS instruments and may or may not be applicable to other forms of secondary ion mass spectrometry (SIMS).

1.2 This guide does not purport to address methods of sample preparation. It is the responsibility of the user to adhere to strict sample preparation procedures in order to minimize contamination and optimize signals. See Guide E1078 and ISO 18116 for sample preparation guidelines.

1.3 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.4 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 ASTM Standards:²

E673 Terminology Relating to Surface Analysis (Withdrawn 2012)³

E1078 Guide for Specimen Preparation and Mounting in Surface Analysis

E1504 Practice for Reporting Mass Spectral Data in Secondary Ion Mass Spectrometry (SIMS)

E1635 Practice for Reporting Imaging Data in Secondary Ion Mass Spectrometry (SIMS)

¹ This practice is under the jurisdiction of ASTM Committee E42 on Surface Analysis and is the direct responsibility of Subcommittee E42.06 on SIMS.

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² For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

³ The last approved version of this historical standard is referenced on www.astm.org.

2.2 ISO Standards:⁴

ISO 23830 Repeatability and Constancy of the Relative Intensity Scale

ISO 18115:2007 Terminology Related to Surface Chemical Analysis

ISO 18116 Guidelines for Preparation and Mounting of Specimens for Analysis

3. Terminology

3.1 *Definitions*—See Terminology E673 and ISO 18115:2007 for definitions of terms used in SIMS.

3.2 Definitions of Terms Specific to This Standard:

3.2.1 *cationization*—the process by which a positively charged ion is formed, whereby a neutral molecule is combined with a cation, usually a metal ion; the resulting peaks are often referred to as cationized peaks.

3.2.2 *deprotonated molecular ion*—a molecule that has lost a proton to form a negative ion.

3.2.3 *exact mass*—measurement of the mass of an ion with sufficient accuracy to provide an unequivocal identification of its elemental and isotopic composition (**1**);⁵ for example, a peak located at m/z 43.0184 in a positive ion mass spectrum is most likely $C_2H_3O^+$ and cannot be $C_3H_7^+$ (m/z 43.0547).

3.2.4 *fragment ion*—the molecular ion, when struck by a primary ion beam, will typically break up into smaller pieces; this process is called fragmentation; a charged dissociation product arising from the fragmentation process is called a fragment ion.

3.2.5 *fragmentation pattern*—the fragmentation of molecular species results in a series of peaks that are characteristic of the molecule's underlying structure; this series of peaks is referred to as the fragmentation pattern of the molecule.

3.2.6 *m/z* —the *X*-axis of a mass spectrum is labeled as m/z , defined as the mass of the ion, in daltons, divided by the charge of the ion, where most ions are singly charged.

⁴ Available from International Organization for Standardization (ISO), 1, ch. de la Voie-Creuse, Case postale 56, CH-1211, Geneva 20, Switzerland, <http://www.iso.ch>.

⁵ The boldface numbers in parentheses refer to a list of references at the end of this standard.