INTERNATIONAL STANDARD

ISO 14975

First edition
2000-12-01

Surface chemical analysis — Information formats

Analyse chimique des surfaces — Protocoles de l'information

Reference number
ISO 14975:2000(E)

ISO copyright office
Case postale 56 • CH-1211 Geneva 20
Tel. + 41 22 749 01 11
Fax + 41 22 749 09 47
E-mail copyright@iso.ch
Web www.iso.ch

Printed in Switzerland

Contents

Page

Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

International Standards are drafted in accordance with the rules given in the ISO/IEC Directives, Part 3.

Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

Attention is drawn to the possibility that some of the elements of this International Standard may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

International Standard ISO 14975 was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 3, *Data management and treatment*.

Annexes A and B of this International Standard are for information only.

Introduction

ISO 14976 provides a digital data transfer format for communicating surface chemical analysis data. Since the importance of databases is increasing in many scientific fields, storage and manipulation of spectral data in databases have become necessary. The structure of ISO 14976 is suitable for communication, but database manipulation is quite different from data communication. Information additional to that contained in ISO 14976 is necessary to handle the data in the databases, so this International Standard proposes three formats which define information packages for (1) specimen information, (2) calibration information and (3) data processing information, which are important to manipulate spectral data in databases. The future compatibility of the format is essential. This format is designed to work with ISO 14976 so that software designed to read the latter will still function correctly with these information packages added. This International Standard, therefore, is supplementary to and compatible with ISO 14976.

The motivation behind the choices made in defining the textual form of the data files described in this International Standard are important. To make it easy for programmers to implement the format reliably in new software, aspects of the Microsoft Windows™ ".INI" file structure are followed. Most modern computers have facilities to read and write this format from a wide range of computer languages via the Windows Application Programming Interface™.

Surface chemical analysis — Information formats

1 Scope

This International Standard specifies a format to supplement ISO 14976 to transfer data for the creation, expansion and revision of a surface chemical analysis spectral database. The format is applied to Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS) spectral data.

2 Normative reference

The following normative document contains provisions which, through reference in this text, constitute provisions of this International Standard. For dated references, subsequent amendments to, or revisions of, any of these publications do not apply. However, parties to agreements based on this International Standard are encouraged to investigate the possibility of applying the most recent edition of the normative document indicated below. For undated references, the latest edition of the normative document referred to applies. Members of ISO and IEC maintain registers of currently valid International Standards.

ISO 14976, *Surface chemical analysis — Data transfer format.*

3 Terms and definitions

For the purposes of this International Standard, the following terms and definitions apply.

3.1
spectral database
set of retrievable spectral data

3.2
information
information about specimens and/or the procedures of analyser calibration and/or data processing procedures and/or the information necessary to create spectral databases

3.3
package
set of text lines which describe information on spectral data

4 Symbols and abbreviated terms

CAS	Chemical Abstracts Service
DTF	data transfer format (as specified in ISO 14976)
IUPAC	International Union of Pure and Applied Chemistry
N/A	not applicable

5 Description of information formats

5.1 General

Information is inserted into the comment lines of the DTF or attached to the DTF as packages. As a result, the existing DTF could be used, without alteration, as a carrier for the information packages; these packages occupy the experiment-comment line or the block-comment lines in the DTF, or build blocks outside the DTF.

With this structure, the reading program, which utilizes information packages, can look for the format identifiers in either the experiment-comment lines, where they apply to all blocks, or in the block-comment lines, where they apply to just one block, or outside the DTF. Existing reading programs would interpret these packages as comments intended for human readers and ignore them.

In this International Standard, the information packages for “specimen information format”, “calibration information format”, and “data processing format” are described. It is a modular structure so that compatibility with software previously written is always maintained.

5.2 Additional rules and definitions

text line: up to 80 characters, followed by carriage return

character: one alternative from the following set comprising the character SPACE and the 7-bit ASCII character set:

‘ ’ | ‘!’ | ‘"’ | ‘#’ | ‘$’ | ‘%’ | ‘&’ | ‘’’ | ‘(’ | ‘)’ | ‘*’ | ‘+’ | ‘,’ | ‘-’ | ‘.’ | ‘/’

| ‘0’ | ‘1’ | ‘2’ | ‘3’ | ‘4’ | ‘5’ | ‘6’ | ‘7’ | ‘8’ | ‘9’ | ‘:’ | ‘;’ | ‘<’ | ‘=’ | ‘>’ | ‘?’

| ‘@’ | ‘A’ | ‘B’ | ‘C’ | ‘D’ | ‘E’ | ‘F’ | ‘G’ | ‘H’ | ‘I’ | ‘J’ | ‘K’ | ‘L’ | ‘M’ | ‘N’ | ‘O’

| ‘P’ | ‘Q’ | ‘R’ | ‘S’ | ‘T’ | ‘U’ | ‘V’ | ‘W’ | ‘X’ | ‘Y’ | ‘Z’ | ‘[’ | ‘\’ | ‘]’ | ‘^’ | ‘_’

| ‘`’ | ‘a’ | ‘b’ | ‘c’ | ‘d’ | ‘e’ | ‘f’ | ‘g’ | ‘h’ | ‘i’ | ‘j’ | ‘k’ | ‘l’ | ‘m’ | ‘n’ | ‘o’

| ‘p’ | ‘q’ | ‘r’ | ‘s’ | ‘t’ | ‘u’ | ‘v’ | ‘w’ | ‘x’ | ‘y’ | ‘z’ | ‘{’ | ‘|’ | ‘}’ | ‘~’

where the vertical bar separates alternatives, given between quotation marks.

carriage return: 7-bit ASCII character CARRIAGE RETURN followed by 7-bit ASCII character LINE FEED

multiple text lines: a set of text lines which identify one item

The decimal sign is given as a point in the format items for computer entry and in examples of verbatim computer entries although, in conformance with the ISO/IEC Directives, Part 3, the decimal sign is given as a comma in the rest of the text.

5.3 The formats

5.3.1 Structures

5.3.1.1 Contents of the specimen information package

The specimen information package consists of the following items shown in bold, on contiguous lines of the text file. Bold items are defined in 5.3.2. All items shall be present and in the order given.

specimen information format identifier

host material

IUPAC chemical name

chemical abstracts registry number

host material composition

bulk purity

known impurities

structure

form of product

supplier

lot number

homogeneity

crystallinity

material family

special material classes

specimen mounting

ex situ preparation

in situ preparation

charge control conditions

specimen temperature

comment on specimen information

end of specimen information format identifier

5.3.1.2 Contents of calibration information package

The calibration information package consists of the following items shown in bold, on contiguous lines of the text file. Bold items are defined in 5.3.2. All items shall be present and in the order given.

calibration information format identifier

energy scale calibration

intensity scale calibration

resolution calibration

end of calibration information format identifier

5.3.1.3 Contents of data processing information package

The data processing information package consists of the following items shown in bold, on contiguous lines of the text file. Bold items are defined in 5.3.2. All items shall be present and in the order given.

data processing information format identifier

data-handling procedure

end of data processing information format identifier

5.3.2 Definition of the items in the formats

5.3.2.1 Specimen information format

Items in bold not defined here are defined in 5.2. Texts in italic characters enclosed by quotation marks are used to code the format, although they do not appear in italics in the formatted data. IUPAC nomenclature and CAS registry number are referred to to code the format.

specimen information format identifier is the **text line**:

"*[ISO_Specimen_Information_Format_1998_October_15]*"

host material is a **text line**. This text line starts with "*host_material*=", followed by a generic description of the specimen. For layered structures, the host material is the "bulk" substance near the surface.

IUPAC chemical name is a **text line**. This text line starts with "*IUPAC_chemical_name*=", followed by the IUPAC chemical name of the host material or, if there is no specification, followed by "*none*", "*unknown*" or "*N/A*".

chemical abstracts registry number is a **text line**. This text line starts with "*chemical_abstracts_registry_number*=", followed by the CAS registry number of the host material or, if there is no specification, followed by "*none*", "*unknown*" or "*N/A*".

host material composition is a **text line**. This text line starts with "*host_material_composition*=", followed by the list of the principal elements present or the chemical formula. When the principal elements' names are used, the composition is given by a real number followed by "*mass%*" or "*atomic%*". If the composition cannot be specified, use "-" instead of a real number.

bulk purity is a **text line**. This text line starts with "*bulk_purity*=", followed by the purity of the material and guarantor (if possible) or, if there is no specification, followed by "*unknown*" or "*N/A*". The purity is given by a real number, and the units acceptable are mass% and atomic%. The units shall be given. An expression like "4N" is not acceptable.

known impurities is a **text line**. This text line starts with "*known_impurities*=", followed by the impurity name(s), concentration(s) and guarantor (if possible) or, if there is no specification, followed by "*none*", "*unknown*" or "*N/A*". The units acceptable are as follows: mass%, atomic%, ppm, ppb, atoms/cm3, and atoms/cm2. The units shall be given.

structure is a **text line**. This text line starts with "*structure*=", followed by information such as a description of the crystal lattice and orientation, e.g. hexagonal close-packed, and/or comments such as fracture surface at grain boundary, etc., or, if there is no specification, followed by "*unknown*" or "*N/A*".

form of product is a **text line**. This text line starts with "*form_of_product*=", followed by the form of the product that the specimen is used for or, if there is no specification, followed by "*unknown*" or "*N/A*".

supplier is a **text line**. This text line starts with "*supplier*=", followed by the name of the manufacturer and/or supplier of the host material or by a reference to how the host was made or, if there is no specification, followed by "*unknown*" or "*N/A*".

lot number is a **text line**. This text line starts with "*lot_number*=", followed by the code that identifies the production run, etc., or, if there is no specification, followed by "*unknown*" or "*N/A*".

homogeneity is a **text line**. This text line starts with "*homogeneity*=", followed by "*homogeneous*" or "*inhomogeneous*" or "*unknown*" or "*N/A*" or another description of the homogeneity of the specimen if none of these is appropriate. This may be followed by a comment, provided the comment is preceded by "*;*".

crystallinity is a **text line**. This text line starts with "*crystallinity*=", followed by "*single*" (single crystal, together with Miller indices of the surface connected by "_") or "*poly*" (polycrystalline) or "*amorphous*" or "*unknown*" or "*N/A*" or another description of the crystallinity of the specimen if none of these is appropriate. This may be followed by a comment, provided the comment is preceded by "*;*".

material family is a **text line**. This text line starts with "*material_family*=", followed by "*metal*" or "*inorganic*" (inorganic compound) or "*organic*" (organic compound) or "*polymer*" or "*semi*" (semiconductor) or "*bio*" (biological material) or "*composite*" or "*super_conductive*" (super-conductive material) or another description of the crystallinity of the specimen if none of these is appropriate. This may be followed by a comment, provided the comment is preceded by "*;*".

special material classes is a **text line**. This text line starts with "*special_material_classes*=", followed by "*rod*" (rod or ingot) or "*sheet*" [sheet or foil (without substrate)] or "*film_single*" [single-layer thin film or coating (on substrate)] or "*film_multi*" [multi-layered thin film or multi-layered coating (on substrate)] or "*sinter*" (sintered material) or "*wafer*" or "*powder*" or "*fibre*" or another description of the special material class of the specimen if none of these is appropriate. This may be followed by a comment, provided the comment is preceded by "*;*".

specimen mounting is a **text line**. This line starts with "*specimen_mounting*=", followed by "*mechanical*" (mechanically mounted using a screw, spring, etc.) or "*mechanically_under_grid*" (mechanically pressed to a grid by a spring) or "*conductive_adhesive*" (fixed by conductive adhesive material) or "*nonconductive_adhesive*" (fixed by non-conducting adhesive material) or "*powder_compact_In*" (powder compact in indium foil, indium pressure pad) or "*powder_put_into*" [powder put into a conductive material (for example, a hole in a copper block)] or another description of the specimen mounting if none of these is appropriate. This may be followed by a comment, provided the comment is preceded by "*;*".

ex situ preparation is a **text line**. This text line starts with "*ex_situ_preparation*=", followed by "*none*" or "*polish*" or "*cleavage*" or "*ion*" (cut by ion beam) or "*powder_compact_steel_pad*" (powder compacted using steel pressure pad) or "*acetone*" (degreased by acetone) or another description of ex situ preparation of the specimen if none of these is appropriate. If ex situ preparation is carried out by a series of the above procedures, **multiple text lines** are used, and the label for each text line is numbered, i.e. "*ex_situ_preparation_1*=", "*ex_situ_preparation_2*=", etc. The number indicates the order of the ex situ preparation procedures. If different kinds of ex situ preparation are carried out simultaneously, the ex situ preparation procedures are combined with "+" following the single label "*ex_situ_preparation*=". The text line may be followed by a comment, provided the comment is preceded by "*;*".