

Australian Standard<sup>®</sup>

## Surface chemical analysis—Information formats



This Australian Standard® was prepared by Committee CH-016, Spectroscopy. It was approved on behalf of the Council of Standards Australia on 20 September 2006. This Standard was published on 20 October 2006.

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- CSIRO Energy Technology
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- Department of Natural Resources and Mines Qld
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- 

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## Surface chemical analysis—Information formats

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## PREFACE

This Standard was prepared by the Standards Australia Committee CH-016, Spectroscopy. This Standard is identical with, and has been reproduced from, ISO 14975:2000, *Surface chemical analysis—Information formats*.

The objective of this Standard is to provide a format to supplement AS/ISO 14976 to transfer data for the creation, expansion and revision of a surface chemical spectral data base.

As this Standard is reproduced from an International Standard, the following applies:

- (a) Its number appears on the cover and title page while the International Standard number appears only on the cover.
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- (c) A full point substitutes for a comma when referring to a decimal marker.

References to International Standards should be replaced by references to Australian or Australian/New Zealand Standards, as follows:

| <i>Reference to International Standard</i>    | <i>Australian Standard</i>                           |
|-----------------------------------------------|------------------------------------------------------|
| ISO                                           | AS ISO                                               |
| 14976 Surface chemical analysis—Data transfer | 14976 Surface chemical analysis—Data transfer format |

The term ‘informative’ has been used in this Standard to define the application of the annex to which it applies. An ‘informative’ annex is only for information and guidance.

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## 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™.

## AUSTRALIAN STANDARD

**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**