Australian Standard®

Surface chemical analysis—Information formats

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- Australian Institute of Physics
- CSIRO Energy Technology
- Department of Defence (Australia)
- Department of Natural Resources and Mines Qld
- National Association of Testing Authorities Australia
- Queensland Health Scientific Services

Additional Interests:

- Curtin University of Technology
- La Trobe University
- University of Newcastle
- The University of New South Wales
- The University of Queensland
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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.

(b) In the source text 'this International Standard' should read 'this Australian Standard'.

(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:

Reference to International Standard		*Australian Standard*	
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