

DRAFT INTERNATIONAL STANDARD

ISO/DIS 22029

ISO/TC 202

Secretariat: SAC

Voting begins on:
2020-01-13

Voting terminates on:
2020-04-06

Microbeam analysis — EMSA/MAS standard file format for spectral-data exchange

Analyse par microfaisceaux — Format de fichier standard EMSA/MAS pour échange de données spectrométriques

ICS: 71.040.99

iTeh STANDARD PREVIEW
(standards.iteh.ai)

[ISO/DIS 22029](#)

<https://standards.iteh.ai/catalog/standards/sist/f5f9689b-5b07-4341-87c5-56b73581eb93/iso-dis-22029>

THIS DOCUMENT IS A DRAFT CIRCULATED FOR COMMENT AND APPROVAL. IT IS THEREFORE SUBJECT TO CHANGE AND MAY NOT BE REFERRED TO AS AN INTERNATIONAL STANDARD UNTIL PUBLISHED AS SUCH.

IN ADDITION TO THEIR EVALUATION AS BEING ACCEPTABLE FOR INDUSTRIAL, TECHNOLOGICAL, COMMERCIAL AND USER PURPOSES, DRAFT INTERNATIONAL STANDARDS MAY ON OCCASION HAVE TO BE CONSIDERED IN THE LIGHT OF THEIR POTENTIAL TO BECOME STANDARDS TO WHICH REFERENCE MAY BE MADE IN NATIONAL REGULATIONS.

RECIPIENTS OF THIS DRAFT ARE INVITED TO SUBMIT, WITH THEIR COMMENTS, NOTIFICATION OF ANY RELEVANT PATENT RIGHTS OF WHICH THEY ARE AWARE AND TO PROVIDE SUPPORTING DOCUMENTATION.

This document is circulated as received from the committee secretariat.



Reference number
ISO/DIS 22029:2020(E)

© ISO 2020

iTeh STANDARD PREVIEW
(standards.iteh.ai)

ISO/DIS 22029

<https://standards.iteh.ai/catalog/standards/sist/f5f9689b-5b07-4341-87c5-56b73581eb93/iso-dis-22029>



COPYRIGHT PROTECTED DOCUMENT

© ISO 2020

All rights reserved. Unless otherwise specified, or required in the context of its implementation, no part of this publication may be reproduced or utilized otherwise in any form or by any means, electronic or mechanical, including photocopying, or posting on the internet or an intranet, without prior written permission. Permission can be requested from either ISO at the address below or ISO's member body in the country of the requester.

ISO copyright office
CP 401 • Ch. de Blandonnet 8
CH-1214 Vernier, Geneva
Phone: +41 22 749 01 11
Fax: +41 22 749 09 47
Email: copyright@iso.org
Website: www.iso.org

Published in Switzerland

Contents

	Page
Foreword	iv
Introduction	v
1 Scope	1
2 General considerations	1
3 Format Description	2
3.1 General.....	2
3.2 Required Keywords.....	3
3.3 Spectral Data.....	4
3.4 Optional Keywords.....	5
3.5 Ending A File.....	9
4 Example Of A Data File In The EMSA/MAS Spectral Format	9
Bibliography	11

iTeh STANDARD PREVIEW (standards.iteh.ai)

[ISO/DIS 22029](#)

<https://standards.iteh.ai/catalog/standards/sist/f5f9689b-5b07-4341-87c5-56b73581eb93/iso-dis-22029>

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 2. The main task of technical committees is to prepare International Standards. 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 document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

ISO 22029 was prepared by Technical Committee ISO/TC 202, *Microbeam analysis*.

This third edition cancels and replaces the second edition (ISO 22029:2012), which has been technically revised.

iTeh STANDARD PREVIEW (standards.iteh.ai)

[ISO/DIS 22029](https://standards.iteh.ai/catalog/standards/sist/f5f9689b-5b07-4341-87c5-56b73581eb93/iso-dis-22029)

<https://standards.iteh.ai/catalog/standards/sist/f5f9689b-5b07-4341-87c5-56b73581eb93/iso-dis-22029>

Introduction

The original EMSA/MAS Standard File Format for Spectral Data Exchange was published in October 1991. Since then, advances in both microbeam analysis techniques and in PC technology have meant that this original standard is not fully able to meet modern requirements. The members of ISO/TC 202 (the International Organization for Standardization Technical Committee for Microbeam Analysis) propose this updated version. Every effort has been made to only make those changes that improve or update the applicability of the standard, while minimizing incompatibility with the original version. The remit of TC 202 does not include surface analysis techniques, which are addressed by TC 201, and so references to these techniques have been removed from the original standard where necessary. The original document also included examples of coding and telecommunications protocols. Since these are now largely outdated, and not integral to the formatting of the data, these have also been removed.

It is noted that one of the originating societies (EMSA) has modified its name since the original document was published. The society is now officially known as the “Microscopy Society of America”, or MSA, the term “Electron” having been dropped to more fully indicate the work and interest of the membership of the society in all forms of microscopy.

Nine new optional user defined keywords have been added to this edition to improve the ability of the standard to more fully describe the instrument and analysis conditions, while still maintaining backward compatibility with data readers and writers conforming with earlier versions of the standard.

iTeh STANDARD PREVIEW (standards.iteh.ai)

[ISO/DIS 22029](https://standards.iteh.ai/catalog/standards/sist/f5f9689b-5b07-4341-87c5-56b73581eb93/iso-dis-22029)

<https://standards.iteh.ai/catalog/standards/sist/f5f9689b-5b07-4341-87c5-56b73581eb93/iso-dis-22029>

iTeh STANDARD PREVIEW
(standards.iteh.ai)

ISO/DIS 22029

<https://standards.iteh.ai/catalog/standards/sist/f5f9689b-5b07-4341-87c5-56b73581eb93/iso-dis-22029>

Microbeam analysis — EMSA/MAS standard file format for spectral-data exchange

1 Scope

This International Standard presents a simple format for the exchange of digital spectral data that has been designated as an EMSA/MAS standard. This format is readable by both humans and computers and is suitable for transmission through various electronic networks, the phone system (with modems) or on physical computer storage devices (such as removable media). The format is not tied to any one computer, programming language or computer operating system. The adoption of a standard format would enable different laboratories to freely exchange spectral data, and would help to standardize data analysis software. If equipment manufacturers were to support a common format, the microscopy and microanalysis community would avoid duplicated effort in writing data analysis software.

2 General considerations

The virtues of a single standard data format have been admirably related by various authors^{[1],[2],[3],[4]}. It would often be convenient, after visiting another laboratory to use a different type of microanalytical spectrometer, to be able to return to one's own laboratory to analyse the data, or for a laboratory to be able to send a spectrum to another group at another location for analysis on their computer. A common format would also enable test spectra to be transported between data acquisition systems, in order to compare different data analysis routines, and would give users greater choice of analysis procedure, based on commercial or public-domain software.

Obviously, an ideal solution would be for the manufacturers to represent data in a standard format, but they are unlikely to agree on this without some direction from their customers (the microanalysis community). Therefore it is highly desirable for EMSA and MAS to proceed with the adoption of a standard format. Such a format does not preclude any research group or manufacturer from having their own, possibly proprietary, format. Spectral data can be stored internally in any format, as long as there is an option to convert it to the external standard (and vice versa) for the purposes of exchange. We believe that a standard format should possess the following attributes:

- a) It should be capable of representing the data exactly (without altering the scientific content).
- b) The format should be simple and easy to use.
- c) It must NOT be tied to any particular computer, programming language or operating system. It should work on a large number of computers of all sizes, although we cannot guarantee that it will work on all possible computers.
- d) The format should be both human and machine (computer) readable.
- e) It should be compatible with existing electronic communication networks and with the phone system (using modems). Future networks will likely retain compatibility with these.
- f) The format should support spectra of interest to the microanalysis community (such as XEDS, EELS, AES) and should be flexible enough to accommodate future data sets not yet specified.
- g) Each file should contain enough information to uniquely identify the type and origin of the spectral data and to reconstruct its significance.
- h) Where possible, the format should be compatible with various commercial data plotting or analysis programs (i.e. spreadsheets, or graphical-analysis packages).

- i) The proposed format need not be the most efficient storage mechanism. Its primary goals, stated above, will generally prevent storage efficiency. If anything, this format will err on the side of simplicity and ease of use.

The format originally employed by the Electron Microscopy and Microanalysis Public Domain Library (EMMPDL) at Argonne^[1] has the virtue of simplicity, but is too rigid for general use. A recent revision^[5] corrected some inadequacies, but a more serious re-examination is in order. The format proposed by a previous EMSA task force^{[3],[4]} addresses many of the problems, but is thought by some microscopists to be too complicated for everyday use. The VAMAS format, whose description^[6] runs to 60 pages, is also too complex for our perceived purpose. A format, named JCAMP-DX, used by the infrared-spectroscopy community^[2] is specific and detailed, but is somewhat off target for the spectroscopies of interest to our community.

The format proposed here follows JCAMP-DX in many ways but is less complicated and has features tailored to X-ray, energy-loss and Auger spectroscopies. We circulated a preliminary version of this proposal to several manufacturers of XEDS systems and have received back comments and suggestions, many of which have been incorporated into this document.

The companion problem of a standard format for digital-image storage is similar to that of spectral data but is sufficiently different to warrant its own standard. Whereas most spectra are sufficiently compact that they can be stored in a human-readable form, image data are usually so extensive as to require storage of "raw" binary numbers. There exist formats for image storage that are in widespread use. One of these (probably TIFF) should be endorsed by EMSA and MAS, allowing the microanalysis community to take advantage of the large amount of commercial and public-domain software already available.

iTeh STANDARD PREVIEW

3 Format Description (standards.iteh.ai)

3.1 General

[ISO/DIS 22029](#)

<https://standards.iteh.ai/catalog/standards/sist/519689b-5b07-4341-87c5-5a7c511b935a>

The general structure of the data file format can be summarized as a simple sequential text file. It begins with a series of header lines which serve to define the characteristics of the spectrum. These header lines are identified by unique keyword fields which occupy the first 15 positions of each line, followed by a data field. These are described in detail below. After the header lines, a keyword indicates the start of data, and the data then follow on successive lines in a manner which is defined explicitly within the header. Finally, after all the data are presented, an end-of-data keyword indicates that the data set is complete. This is diagrammatically illustrated below:

Header lines

- *
- *

Successive lines beginning with EMSA/MAS-defined keywords, some of which are required and some are optional

- *
- *

Start-of-data keyword

- *
- *

Experimental data

- *

*

End-of-data keyword

In general, each line of the file either contains a keyword and its associated value or spectral data. All header lines are readily identified as they each begin with “#” in the first character field or column. This symbol demarks the start of a 13 character keyword field, providing descriptive information about the data followed by an associated value. EMSA/MAS-defined keywords (whose definition may be changed only by EMSA/MAS) begin with a single # and occupy the first 13 columns (characters) of each header line. The keyword itself consists of at most 12 characters, which directly follow the #. Shorter

keywords may be employed, and any remaining spaces following the defined keyword may be filled with descriptive text such as unit designation for ease of legibility when the file is printed (see example in Table 1). If a position in the keyword field is not used, it must be filled with a space character. The keywords are not case-sensitive, so that #Xunits is interpreted as being the same as #XUNITS.

The 14th and 15th character positions (columns) in each header line are occupied by keyword/value field separators, which consist of a colon followed by a space. The value associated with each keyword starts in column 16 and may be either textual or numeric as defined by the keyword. Each line of the file may contain no more than 79 characters (for compatibility with the largest number of computers and computer networks, and for general legibility on standard-width CRT screens). Since the keyword and its separator occupies the first 15 positions, this means that all remaining information following the keyword is limited to a maximum of 64 (79 – 15) character positions. The end-of-line indicator is a carriage return/linefeed combination (<CR><LF>).

The only characters allowed in the file, except where explicitly stated, are the space (ASCII character 32), carriage return (ASCII character 13) and linefeed (ASCII character 10) characters, plus the printable ASCII character set given below:

!"#\$%&'()*+,-./0123456789:;< = > ? @ (ASCII characters 33 - 64)

ABCDEFGHIJKLMNOPQRSTUVWXYZ (ASCII characters 65 - 90)

abcdefghijklmnopqrstuvwxyz (ASCII characters 97 - 122)

[\] ^ _ { } approximately (ASCII characters 91 - 96, ASCII 123 - 126)

Horizontal TAB characters are NOT permitted in this file format as a substitute for spaces or commas. Examples of keywords, separators and data can be found in Table 1, and are further detailed below. The file should be named using the extension .TXT, .EMSA or .MSA.

3.2 Required Keywords

The following keywords are required and must appear at the beginning of the file, in the order specified below. Although some of these may appear arbitrary, it is our judgment that they fulfil a long-term need. After several years of students and outside users passing through a laboratory, the result can be a vast number of data files of unknown origin. Unless some adequate form of labelling is imposed from the start, many worthwhile data files are lost, and useless data sit on a disc taking up valuable space. With the following minimum subset of keywords, it should be possible to reconstruct the significance of most spectra.

Note that there must be exactly one of each required keyword, except for the keyword #TITLE which must appear at least once but may, at the user's discretion, appear more than once to provide an extended-length title.

Required keywords: