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Surface chemical analysis — Data transfer format

Analyse chimique des surfaces — Protocole pour le transfert des données

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Contents		
	The Components of the metalanguage Additional rules	- - - - - - - - - - - - - - - - - - -
Annex	A Design of the format	14
Annex B B B	.1 General	16 16 16 18
Annex C C	,	2! 2! 2!
С	3 An experiment involving a number of regularly-scanned spectral regions as a function of sputtering as in a sputter depth profile by one technique such as AES or SIMS, the analysis not being at a particularly addressed point on the sample	30
C	An experiment involving a number of maps of single values representing the intensities of different elements for one technique such as AES, EDX or SIMS, the maps to be made of x-linescans starting at (1,1) and varying with one experimental variable.	35
Annex	D Bibliography	41

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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 nongovernmental, 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.

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.

International Standard ISO 14976 was prepared by Technical Committee ISO/TC 201, Surface chemical analysis, Subcommittee 3, Data management and treatment.

Annexes A to D of this International Standard are for information only.

Introduction

In surface analysis many commercial instruments are operated through a computer. This computer is also used for processing the captured data, using routines from a built-in set of options for peak synthesis, peak deconvolution, background subtraction, peak area measurement, quantification in various levels of sophistication, mapping, depth profile presentation, smoothing, differentiation and a host of other functions. However, many analysts wish to process their data on another computer in their own particular way using programs written to their specification and under their full control. They need to encode the data in the data-capture computer into a form suitable for transmission then decode it into the form required in the receiving computer. Manufacturer's data formats all differ and differ again from instrument model to instrument model for any given manufacturer. These formats are not published. A standard format for the transferring of data is required to enhance communication, reduce the number of programs required to effect the encoding and decoding and to reduce the uncertainty of data analysis.

iv

Surface chemical analysis — Data transfer format

1 Scope

This International Standard specifies a Format to transfer data from computer to computer via parallel interfaces or via serial interfaces over direct wire, telephone line, local area network or other communications link. The transferred data is encoded only in those characters that appear on a normal display or printer. The format is suitable for AES, EDX, FABMS, ISS, SIMS, SNMS, UPS, XPS, XRF and similar analytical methods. It covers spectra, elemental maps, depth profiles and sequences of data resulting from a variety of experiments.

2 Description of the format

2.1 General

The design of this Format is presented in Annex A. The Format is described using components of the metalanguage defined in the British Standard - Method of defining syntactic metalanguage, BS 6154:1981⁽¹⁾, the appropriate elements of which are given in 2.2 and 2.3.

In this Format some parameters are relevant only to particular cases of the three items; experiment mode, scan mode or technique, and provision is made for including these parameters only where they are relevant. This conditional inclusion could be expressed in the metalanguage, but only at the expense of a more complicated structure than a simple list. To keep the structure simple these parameters are expressed as optional-sequences, and have the conditions under which each of these optional-sequences is to be included specified in an accompanying bracketed-textual-comment.

2.2 The Components of the metalanguage

The metalanguage comprises a notation for specifying a set of rules for generating a linear sequence of characters. Only characters generated by the rules are to be inserted in the sequence. The sequence may be considered as being a sequence of sub-sequences. A sub-sequence may be represented in the notation by enclosing the given characters within either a pair of APOSTROPHE or a pair of QUOTATION MARK characters. The sub-sequence together with these enclosing characters is called a terminal-string.

A terminal-string is one example of a syntactic-primary.

A syntactic-primary may be preceded by an integer followed by an ASTERISK to represent a specific number of successive occurrences of the same syntactic-primary. A syntactic-primary, together with a preceding integer and ASTERISK, if present, is called a *syntactic-factor*.

A syntactic-factor may be followed by a MINUS SIGN followed by another syntactic-factor. This sub-sequence is called a syntactic term.

A number of syntactic-terms may be given in succession but separated by COMMA characters to represent a sub-sequence generated by applying each of the syntactic-terms in turn. A single syntactic-term or group of syntactic-terms separated by COMMA characters is called a *single-definition*.

A number of single-definitions may be given in succession but separated by VERTICAL LINE characters to represent the generation of a sub-sequence by one and only one of the single-definitions, that is, to represent a list of alternative single-definitions. A single-definition or group of single-definitions separated by VERTICAL LINE characters is called a definitions-list.

What is represented by the MINUS SIGN followed by a second syntactic-factor when present in a syntactic-term may now be explained. It is to except from generation by the syntactic-term any sub-sequence that could be generated by the second syntactic-factor. The second syntactic-factor is called a *syntactic-exception*.

A unique name may be assigned to a particular definitions-list. The name may consist of one or more characters. The first character must be a letter. Any subsequent character may be a letter or a digit. Spaces and new lines included in the name are not significant. The name is called a *meta-identifer*.

A meta-identifier is assigned to a definitions-list by giving the meta-identifier followed by an EQUALS SIGN followed by the definitions-list followed by a SEMICOLON. This is called a *syntax-rule*.

One or more syntax-rules together make up the set of rules for generating the linear sequence of characters. The set of rules is called a syntax.

A syntactic-primary, which has been introduced as having a terminal-string as an example, may now be defined as consisting of one of the following:

- (a) No characters at all, representing no characters being added to the sequence. This is called an *empty-sequence*.
- (b) A LEFT BRACKET followed by a definitions-list followed by a RIGHT BRACKET, representing the generation of either an empty-sequence or one sub-sequence represented by the definitions-list. This is called an *optional-sequence*.
- (c) A LEFT BRACE followed by a definitions-list followed by a RIGHT BRACE, representing either an empty-sequence or a succession of any number of sub-sequences each of which is a sub-sequence that may be generated by the definitions-list. This is called a *repeated-sequence*.
- (d) A LEFT PARENTHESIS followed by a definitions-list followed by a RIGHT PARENTHESIS, representing any sub-sequence generated by the enclosed definitions-list. This is called a grouped-sequence.

- (e) A meta-identifier, already described, representing any sub-sequence generated by the definitions-list to which it has been assigned in a syntax-rule.
- (f) A terminal-string, already described, representing the enclosed sub-sequence.
- (g) A QUESTION MARK followed by some text followed by another QUESTION MARK, representing a sub-sequence that is described in the enclosed text in another language because it cannot be represented in the metalanguage itself. This is called a special-sequence.

The characters LEFT PARENTHESIS and ASTERISK followed by some text followed by the characters ASTERISK and RIGHT PARENTHESIS is called a *bracketed-textual-comment*. This allows a comment for the benefit of the human reader to be added to a syntax without affecting its meaning. It may be inserted anywhere in a syntax except in a meta-identifier, an integer, a special-sequence or a terminal-string.

With the exception of terminal-strings the layout on the page does not affect the meaning of the syntax.

- NOTE 1 The following is a summary of the special symbols of the metalanguage. The first six are given in the order of precedence implied in the description of 2.2 with highest precedence at the top, this order being overridden by the bracket-pairs that follow them.
- * follows an integer specifying the number of occurrences of the following syntactic-primary in a syntactic-factor.
- precedes a syntactic-exception in a syntactic-term.
- , separates successive syntactic-terms in a single-definition.
- separates alternative single-definitions in a definitions-list.
- = separates the definitions-list from the meta-identifier being defined in a syntax-rule.
- ; terminates a syntax-rule.
- ' and ' or
- " and " enclose characters to form a terminal-string, representing the characters as they are generated.
- (* and *) enclose a comment to form a bracketed-textual-comment, giving additional information for the human reader.
- (and) enclose a definitions-list to form a grouped-sequence, grouping items together in the usual algebraic sense.
- { and } enclose a definitions-list to form a repeated-sequence, a syntactic-primary which may occur zero or more times.
- [and] enclose a definitions-list to form an optional-sequence, a syntactic-primary which may be omitted or included once.
- ? and ? enclose text to form a special-sequence, a syntactic-primary described in a language other than the metalanguage.

2.3 Additional rules

Some parameters need to be repeated a number of times, the actual number of repeats depending on the value of a parameter that has occurred earlier in the format. There is no provision in the metalanguage for expressing this dependence. In these cases the parameters are expressed as repeated-sequences, and the name of the parameter whose value gives the actual number of repeats is given in an accompanying bracketed-textual-comment.

A real number equal to 1E37 is to be taken as a dummy value indicating that the true value is not known. The only integer values that may not be known are those specifying elements of date or time of day and in these cases the value -1 is used as a dummy value.

NOTE 2 Where meta-identifiers are used inside bracketed-textual-comments they are printed in italics.

NOTE 3 Each meta-identifier in the definitions-lists in the syntax-rules defining experiment and block corresponds to a simple-variable or array-variable stored in the data-capture computer. When output in the Format each variable or array-element is represented by a sub-sequence ending in a carriage return composed of the ASCII characters with denary values 13 and 10, the widely-used CARRIAGE RETURN LINE FEED combination. The sub-sequence forms a normal integer or real-number representation of a stored numerical value or expresses an equivalent stored text string. Each of the meta-identifiers consists of a word or phrase chosen to be unambiguous, and additional explanation of its

meaning is given in a bracketed-textual-comment where necessary. These two syntax-rules have been given first, followed by the remaining syntax-rules in alphabetical order.

The format

experiment = format identifier, institution identifier, instrument model identifier, operator identifier, experiment identifier, number of lines in comment,

{comment line}

(* The number of occurrences of comment line is specified by the value of number of lines in comment above.

The comment may include details of the last calibration of the instrument. *).

experiment mode,

scan mode,

[number of spectral regions]

(* Normally only one technique is used in an experiment but there may be more. The value of number of spectral regions is the sum for all techniques of the numbers of spectral regions in each technique. number of spectral regions is inserted if and only if the value of experiment mode is 'MAP', 'MAPDP', 'NORM' or 'SDP'. *),

[number of analysis positions,

number of discrete x coordinates available in full map,

number of discrete y coordinates available in full map]

(* The above three entries are inserted if and only if the value of experiment mode is either 'MAP' or 'MAPDP'.

Note that if the product of the values of number of discrete x coordinates available in full map and number of discrete y coordinates available in full map is greater than the value of number of analysis positions then some positions in the map are left empty. *),

number of experimental variables

(* An experimental variable is a parameter which may be varied from block to block through the experiment but which remains constant within each block. *),

{experimental variable label,

experimental variable units)

(* The number of occurrences of the above pair of entries is specified by the value of number of experimental variables above. *),

'0', carriage return,

number of manually entered items in block, {prefix number of manually entered item}

> (* The number of occurrences of prefix number of manually entered item is specified by the value of number of manually entered items in block above. If this is greater than zero then the values of successive occurrences of prefix number of manually entered item should be in ascending order. Any of the items preceded by prefix numbers in comment brackets in the syntax-rule defining block which need to be evaluated by the operator and manually entered from the keyboard should be included in this list. If an item is to be expressed as a real number and the operator is unable to supply a value then the computer should enter the value 1E37. *),

number of future upgrade experiment entries,

number of future upgrade block entries

(* number of future upgrade experiment entries and number of future upgrade block entries are included in case the Format is upgraded in the future to include more non-optional, non-repeating parameters. The numbers of these new parameters will be entered here so that old programs can skip the new parameters in new data, and new programs will not try to read the new parameters in old data. For the present both of them would be set to zero. *),

(future upgrade experiment entry)

(* The number of occurrences of future upgrade experiment entry is given by the value of number of

4

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future upgrade experiment entries above. It is defined as a text line so that any integer, real number or text line inserted here by a future upgrade of the Format can be read as a text line then discarded. *), number of blocks,
```

{block} -

(* The minus-sign followed by the empty-sequence, that is, nothing but the separator, indicates that there must be at least one block.

The number of occurrences of block is specified by the value of number of blocks above. *), experiment terminator;

block = block identifier,

sample identifier,

(* 1*) [year in full]

(* Gregorian calendar year, for example, '1987' *),

(* 2*) [month],

(* 3*) [day of month],

(* 4*) [hours]

(* 24-hour clock *),

(* 5*) [minutes],

(* 6*) [seconds]

(* If the value of any of the above six items is not known the value -1 should be entered as a dummy value. *),

(* 7*) [number of hours in advance of Greenwich Mean Time],

(* 8*) [number of lines in block comment,

(* 8*) {comment line}]

(* The number of occurrences of comment line is specified by the value of number of lines in block comment above. *),

(* 9*) [technique],

(*10*) [x coordinate

(* the ordinal number, starting with unity, of the point in the array along the analysis source deflection system x-axis *),

(*10*) y coordinate]

(* the ordinal number, starting with unity, of the point in the array along the analysis source deflection system y-axis.

The above two entries are inserted if and only if the value of experiment mode is either 'MAP' or 'MAPDP'.*),

(*11*) (value of experimental variable)

(* value of experimental variable may be, for example, total time in seconds, total sputtering time in seconds, total sputtering fluence in ions per m², temperature in Kelvin, energy in electron volts or mass in unified atomic mass units. Where this variable changes smoothly with time this value shall be the value at the start of recording the block data unless specified otherwise in the experimental variable label.

The number of occurrences of value of experimental variable is specified by the value of number of experimental variables above, and the order in which the values are given is the same as the order in which experimental variable label and experimental variable units are declared above. *),

(*12*) [analysis source label],

(*13*) [sputtering ion or atom atomic number,

(*13*) number of atoms in sputtering ion or atom particle,

(*13*) sputtering ion or atom charge sign and number]

(* The above three entries are inserted if and only if either (1) the value of experiment mode is 'MAPDP', 'MAPSVDP', 'SDP' or 'SDPSV', or (2) the value of technique is 'FABMS', 'FABMS energy spec', 'ISS', 'SIMS', 'SIMS energy spec', 'SNMS' or 'SNMS energy spec'.*),

(*14*) [analysis source characteristic energy]

(* energy in electron volts *),

(*15*) [analysis source strength]

(* power in watts for XPS and XRF; beam current in nanoamps for AES, EDX, ISS, SIMS and SNMS; beam equivalent for FABMS *),

(*16*) [analysis source beam width x

(* width in micrometres at the sample in the plane perpendicular to the source beam *),

(*16*) analysis source beam width y]

(* width in micrometres at the sample in the plane perpendicular to the source beam*),

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ISO 14976:1998(E)
 (*17*)
            ffield of view x
               (* micrometres *).
 (*17*)
            field of view yl
               (* micrometres.
                  The above two entries are inserted if and only if the value of experiment mode is 'MAP', 'MAPDP',
               'MAPSV', 'MAPSVDP' or 'SEM'. *),
 (*18*)
           [first linescan start x coordinate,
 (*18*)
           first linescan start y coordinate,
 (*18*)
           first linescan finish x coordinate,
 (*18*)
           first linescan finish y coordinate,
 (*18*)
           last linescan finish x coordinate,
 (*18*)
           last linescan finish y coordinate]
              (* The above six entries are inserted if and only if the value of experiment mode is 'MAPSV', 'MAPSVDP'
              or 'SEM'.
                  They are required for specifying the size and shape of the map and for relating the order in the scan sequence
              to the position on the sample.
                  In the coordinate system to be used, x-values start at unity at the left-hand side of the frame and increase
              towards the right-hand side, and y-values start at unity at the top of the frame and increase towards the bottom
              of the frame, as shown below.
                   1.1
                                   N.1
                                  N<sub>.</sub>M
                   1.M
(*19*)
           [analysis source polar angle of incidence]
```

(* degrees from upward z-direction, defined by the sample stage *),

(*20*)[analysis source azimuth]

(* degrees clockwise from the y-direction, defined by the sample stage*),

(*21*)[analyser mode],

(*22*)[analyser pass energy or retard ratio or mass resolution]

(* energy in electron volts, mass in amu *),

(*23*)[differential width]

(* electron volts peak-to-peak for sinusoidal modulation or computer differentiation.

differential width is inserted if and only if the value of technique is 'AES diff'. *),

[magnification of analyser transfer lens], (*24*)

(*25*)[analyser work function or acceptance energy of atom or ion]

(* positive value for work function in electron volts for AES, ELS, ISS, UPS and XPS. The acceptance energy of an ion is the energy filter pass energy of the mass spectrometer for FABMS, SIMS, and SNMS. *).

(*26*)[target bias]

(* target bias is in volts, including the sign. *),

(*27*)[analysis width x

> (* The analysis width x is the gated signal width of the source in the x-direction in the plane perpendicular to the beam for FABMS, FABMS energy spec, ISS, SIMS, SIMS energy spec, SNMS and SNMS energy spec, the analyser slit length divided by the magnification of the analyser transfer lens to that slit for AES diff, AES dir, ELS, UPS and XPS, and is the source width in the x-direction for both EDX and XRF.

analysis width x is in micrometres. *),

(*27*)analysis width y]

(* As analysis width x but for y. *),

(*28*)[analyser axis take off polar angle

(* degrees from upward z-direction, defined by the sample stage *),

6

```
(*28*)
            analyser axis take off azimuth]
               (* degrees clockwise from the y-direction, defined by the sample stage*),
 (*29*)
            [species label]
               (* elemental symbol or molecular formula *),
 (*30*)
            [transition or charge state label
               (* for example, 'KLL' for AES, '1s' for XPS, '-1' for SIMS *),
 (*30*)
            charge of detected particle]
               (* for example, -1 for AES and XPS, +1 for positive SIMS *),
 (*31*)
           [abscissa label,
 (*31*)
           abscissa units,
 (*31*)
           abscissa start,
 (*31*)
           abscissa increment]
               (* The above four entries are inserted if and only if the value of scan mode is 'REGULAR'.*),
 (*32*)
           [number of corresponding variables
               (* If the data is in the form of sets of corresponding values of two or more variables then number of
               corresponding variables is equal to the number of variables, otherwise it is equal to unity. *),
 (*32*)
           (corresponding variable label,
 (*32*)
           corresponding variable units] ]
              (* The number of occurrences of the above pair of items is specified by the value of number of corresponding
              variables above. *),
 (*33*)
           [signal mode],
 (*34*)
           [signal collection time]
              (* time in seconds per scan for each channel or array-point, except for both EDX and XRF where it is the total
              spectrum collection time *),
 (*35*)
           [number of scans to compile this block],
(*36*)
           [signal time correction]
              (* This is the system dead time, except for EDX and XRF where it is the livetime-corrected acquisition time.
              In the case of a dead time, a positive value indicates that the count rate should be corrected by dividing by
              (1 - measured rate x dead time) whereas a negative value indicates a correction by multiplying by (exp(true count
              rate x dead time)). If the spectra have already been corrected for dead time the value here will be zero and the
              value of the dead time used will be noted in a comment line or elsewhere.
                signal time correction is in seconds. *),
(*37*)
           [sputtering source energy
              (* energy in electron volts *),
(*37*)
           sputtering source beam current
              (* current in nanoamps or equivalent for neutrals *),
(*37*)
           sputtering source width x
              (* width in micrometres at the sample in the plane perpendicular to the sputtering source beam*),
          sputtering source width y
(*37*)
              (* width in micrometres at the sample in the plane perpendicular to the sputtering source beam*),
(*37*)
          sputtering source polar angle of incidence
              (* degrees from upward z-direction, defined by the sample stage *).
(*37*)
          sputtering source azimuth
             (* degrees clockwise from the y-direction, defined by the sample stage*),
(*37*)
          sputtering mode]
              (* The value of sputtering mode is either 'continuous', when sputtering continues while spectral data is being
              recorded, or 'cyclic', when sputtering is suspended while spectral data is being recorded.
                 The above seven entries are for a sputtering source used in addition to the analysis source, as in depth
             profiling, in AES diff, AES dir, EDX, ELS, UPS, XPS or XRF.
                 The above seven entries are inserted if and only if both (1) the value of technique is 'AES diff', 'AES dir',
              'EDX', 'ELS', 'UPS', 'XPS' or 'XRF', and (2) the value of experiment mode is 'MAPDP', 'MAPSVDP', 'SDP'
             or 'SDPSV'. *),
(*38*)
          [sample normal polar angle of tilt
             (* degrees from upward z-direction, defined by the sample stage *),
(*38*)
          sample normal tilt azimuth]
             (* degrees clockwise from the y-direction, defined by the sample stage*),
```

(*39*) [sample rotation angle]

(* degrees clockwise rotation about the sample normal. If this is referenced to a particular direction on the sample this direction would be specified in a comment line at item number 8.*),

(*40*) [number of additional numerical parameters],

(*40*) (additional numerical parameter label,

(*40*) additional numerical parameter units,

(*40*) additional numerical parameter value)

(* The number of occurrences of the above group of three entries is specified by the value of number of additional numerical parameters above. *),

{future upgrade block entry}

(* The number of occurrences of future upgrade block entry is given by the value of number of future upgrade block entries above. It is defined as a text line so that any integer, real number or text line inserted at this point by a future upgrade of the Format can be read as a text line then discarded. *),

number of ordinate values

(* The value of number of ordinate values is equal to product of the value of number of corresponding variables and the number of sets of corresponding variables to be transferred.*),

(minimum ordinate value,

maximum ordinate value}

(* The number of occurrences of the above pair of entries is specified by the value of number of corresponding variables above. The order in which the pairs of entries appear is the same as the order in which the corresponding values of corresponding variable label are given above. *),

{ordinate value} -

(* The number of occurrences of ordinate value is specified by the value of number of ordinate values above. If the value of number of corresponding variables is greater than unity then the data is sent in the form of successive complete sets, each set consisting of an ordinate value for each of the corresponding variables arranged in the same order as that in which each value of corresponding variable label is given above.

The minus-sign followed by the empty-sequence indicates that there must be at least one ordinate value. *);

abscissa increment = real number

(* For units see the table under abscissa start. *);

abscissa label = text line;

abscissa start = real number;

abscissa units = units

(* The table below shows the usual values of abscissa units for values of technique and experiment mode as a guide but is not mandatory.

	units corresponding to technique			
experiment mode	AES diff, AES dir, EDX, ELS, ISS, UPS, XPS, XRF	FABMS, SIMS, SNMS	FABMS energy spec, SIMS energy spec, SNMS energy spec	
MAP MAPDP NORM SDP	'eV'	'u' or 's'	'eV'	
SDPSV	's'	's'		

*);

additional numerical parameter label = text line;

additional numerical parameter units = units;

additional numerical parameter value = real number;

analyser axis take off azimuth = real number;

analyser axis take off polar angle = real number;

analyser mode = ('FAT' | 'FRR' | 'constant delta m' | 'constant m/delta m'), carriage return;

analyser pass energy or retard ratio or mass resolution = real number;

```
analyser work function or acceptance energy of atom or ion = real number;
 analysis source azimuth = real number;
 analysis source beam width x = real number;
 analysis source beam width y = real number;
 analysis source characteristic energy = real number;
 analysis source label = text line;
 analysis source polar angle of incidence = real number;
 analysis source strength = real number;
 analysis width x = real number,
 analysis width y = real number;
 block identifier = text line;
carriage return = ? 7-bit ASCII character CARRIAGE RETURN followed by 7-bit ASCII character LINE FEED?;
               ' ' | '!' | '"' | '#' | '$' | '%' | '&' | "'"
character =
                                                            | '(' | ')' | '*'
                                                                             1'+' | ','
                                                                       1 ':'
                                                | '6' | '7'
               '0' | '1' | '2' | '3' | '4' | '5'
                                                           1 '8' 1 '9'
               '@' | 'A' | 'B' | 'C' | 'D' | 'E' | 'F' | 'G' | 'H' | 'I' | 'J' | 'K' | 'L' | 'M' | 'N' | 'O'
                   | 'Q' | 'R' | 'S' | 'T' | 'U' | 'V' | 'W' | 'X' | 'Y' | 'Z' | 'I' | \^
                                                                                        | ']' | '^'
                    | 'a' | 'b' | 'c' | 'd' | 'e' | 'f' | 'g' | 'h' | 'i' | 'j' | 'k' | 'l' | 'm' | 'n'
              | 'p' | 'q' | 'r' | 's' | 't'
                                           | 'u' | 'v' | 'w' | 'x' | 'y' | 'z' | '(' | '|' | ')' |
             (* A character is the character SPACE or any of the 94 graphic characters specified in the American National
             Standard for Information Systems - Coded character sets - 7-bit American national standard code for information
             interchange (7-Bit ASCII), ANSI X3.4-1986. 7-bit ASCII is the American national version of the International
             Standard - Information processing - ISO 7-bit coded character set for information interchange, ISO 646-1983.
             or '~'.*);
charge of detected particle = integer;
comment line = text line;
corresponding variable label = text line;
corresponding variable units = units;
day of month = integer;
decimal number = [sign], [ {digit}, '.'], {digit} -
          (* The minus-sign followed by the empty-sequence indicates that there must be at least one digit in decimal
          number.*);
differential width = real number;
digit = '0' | '1' | '2' | '3' | '4' | '5' | '6' | '7' | '8' | '9';
experiment identifier = text line;
experiment mode = ( 'MAP' | 'MAPDP' | 'MAPSV' | 'MAPSVDP' | 'NORM' | 'SDP' | 'SDPSV' | 'SEM'),
          carriage return
          (* The contents of each block in the experiment are indicated by the values of experiment mode as follows:
          'MAP'
                         A spectrum which refers to a specified point in a regular two-dimensional spatial array.
          'MAPDP'
                         A spectrum which refers to a specified point in a regular two-dimensional spatial array and to a
                         specified layer in a depth profile.
          'MAPSV'
                         A complete set of single values of a fixed number of variables for every point in a regular
                         two-dimensional spatial array. Note that an x linescan consists of a map with the value of number
                         of analysis positions equal to the value of number of discrete x coordinates available in full map,
                         that is, the number of discrete y coordinates is unity; in a y linescan the rôles of x and y are
                         reversed.
          'MAPSVDP'
                         A complete set of single values of a fixed number of variables for every point in a regular
                         two-dimensional array for one layer in a depth profile. Successive blocks refer to successive layers
                         in the depth profile.
          'NORM'
                         Either independent data or data which refers to a specified set of single values of one or more
                        experimental variables; the data may be spectral or non-spectral.
          'SDP'
                         A spectrum which refers to a specified layer in a depth profile.
          'SDPSV'
                         A complete set of single values of a fixed number of variables for every layer in a depth profile,
          'SEM'
                        An electron emission intensity for every point in a regular two-dimensional spatial array.
           *);
experiment terminator = 'end of experiment', carriage return;
```

```
experimental variable label = text line;
 experimental variable units = units;
 field of view x = real number;
 field of view y = real number;
 first linescan finish x coordinate = integer;
 first linescan finish y coordinate = integer;
 first linescan start x coordinate = integer:
 first linescan start y coordinate = integer;
 format identifier = 'VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4', carriage return:
 future upgrade block entry = text line;
future upgrade experiment entry = text line;
hours = integer;
institution identifier = text line;
instrument model identifier = text line;
integer = [sign], (digit) -, carriage return
         (* The value of integer must be in the range -1E37 to 1E37.
            The minus-sign followed by the empty-sequence indicates that there must be at least one digit in integer. *);
last linescan finish x coordinate = integer;
last linescan finish y coordinate = integer;
magnification of analyser transfer lens = real number;
maximum ordinate value = real number;
minimum ordinate value = real number;
minutes = integer;
month = integer;
number of additional numerical parameters = zero or more;
number of analysis positions = one or more;
number of atoms in sputtering ion or atom particle = one or more;
number of blocks = one or more;
number of corresponding variables = one or more;
number of discrete x coordinates available in full map = one or more;
number of discrete y coordinates available in full map = one or more;
number of experimental variables = zero or more;
number of future upgrade block entries = zero or more:
number of future upgrade experiment entries = zero or more:
number of hours in advance of Greenwich Mean Time = real number;
number of lines in block comment = zero or more;
number of lines in comment = zero or more;
number of manually entered items in block = zero or more;
number of ordinate values = one or more;
number of scans to compile this block = one or more;
number of spectral regions = one or more;
one or more = integer
        (* The value of one or more must be greater than zero. *);
operator identifier = text line;
ordinate value = real number;
prefix number of manually entered item = one or more;
real number = decimal number, [ 'E', [sign], (digit) - ], carriage return
        (* The value of real number must be in the range -1E37 to -1E-37, or zero, or in the range 1E-37 to 1E37.
           The minus-sign followed by the empty-sequence indicates that the exponent part, if present, must contain at least
        one digit. *);
sample identifier = text line;
sample normal polar angle of tilt = real number;
sample normal tilt azimuth = real number:
sample rotation angle = real number;
scan mode = ( 'REGULAR' | 'IRREGULAR' | 'MAPPING' ), carriage return
        (* If the value of experiment mode is 'MAPSV', 'MAPSVDP' or 'SEM' then the value of scan mode must be
```

'MAPPING', otherwise if the data is in the form of an abscissa start, an abscissa increment and a number of complete

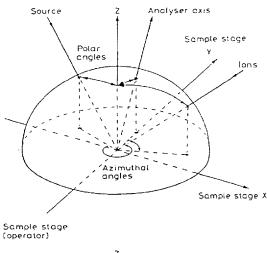
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```
sets of values of one or more experimental variables then the value of scan mode is 'REGULAR', otherwise the value
         of scan mode is 'IRREGULAR'. *);
seconds = integer:
sign = '+' | '-';
signal collection time = real number;
signal mode = ('analogue' / 'pulse counting'), carriage return
         (* Analogue signals, while recorded digitally, may be of either sign and have a gain which may be noted in the block
         comment. Pulse counting signals are integers with values equal to or greater than zero. *);
signal time correction = real number;
species label = text line;
sputtering ion or atom atomic number = one or more;
sputtering ion or atom charge sign and number = integer;
sputtering mode = ( 'continuous' | 'cyclic' ), carriage return;
sputtering source azimuth = real number;
sputtering source beam current = real number;
sputtering source energy = real number;
sputtering source polar angle of incidence = real number;
sputtering source width x = real number;
sputtering source width y = real number;
target bias = real number;
technique = ('AES diff' | 'AES dir' | 'EDX' | 'ELS' | 'FABMS' | 'FABMS energy spec' | 'ISS' | 'SIMS' | 'SIMS
        energy spec' | 'SNMS' | 'SNMS energy spec' | 'UPS' | 'XPS' | 'XRF' ), carriage return;
        (* these techniques are as follows
             AES diff
                                  differentiated Auger electron spectroscopy
             AES dir
                                  direct Auger electron spectroscopy
             EDX
                                  energy dispersive X-ray spectroscopy
             ELS
                                  electron energy loss spectroscopy
             FABMS
                                  fast atom bombardment mass spectroscopy
             ISS
                                  ion scattering spectroscopy
             SIMS
                                  secondary ion mass spectroscopy
             SNMS
                                  sputtered neutral mass spectroscopy
                                  ultra-violet photoelectron spectroscopy
             UPS
             XPS
                                  X-ray photoelectron spectroscopy
             XRF
                                  X-ray fluorescence spectroscopy
        *);
text line = 80*[character], carriage return;
transition or charge state label = text line;
units = ('c/s' | 'd' | 'degree' | 'eV' | 'K' | 'micro C' | 'micro m' | 'm/s' | 'n' | 'nA' | 'ps' | 's' | 'u' | 'V'), carriage
        (* These values are abbreviations for the units listed below:
             'c/s'
                                  counts per second
             'd'
                                  dimensionless - just a number, eg, counts per channel
             'degree'
                                  angle in degrees
             'eV'
                                  electron volts
             'Κ'
                                  Kelvin
             'micro C'
                                 microcoulombs
             'micro m'
                                 micrometres
             'm/s'
                                 metres per second
             'n
                                 not defined here - may be given in a label
             'nA'
                                 nanoamps
             'ps'
                                 picoseconds
             's'
                                 seconds
             'u'
                                 unified atomic mass units
             v.
                                 volts
          *);
```

2.5 Specification of the spectrometer geometry

All angles of the analysis source, the analyser axis, the sputtering source and the sample are defined in figure 1, referred to the fixed orthogonal co-ordinate system of the sample stage x, y and z shift directions. If the sample has no x, y and z stage, the z direction is taken as the upward vertical, the x direction is the direction in the horizontal plane to the operator's right and the y direction is in the same horizontal plane but away from the operator when standing in front of the instrument. The choice of the front may be arbitrary but shall be clearly defined at the time the system geometry is evaluated.



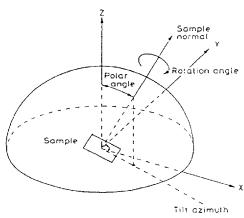


Figure 1 - The relationships of geometrical orientations for specifying angular values.

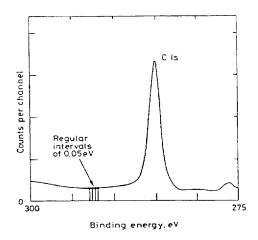


Figure A.1 - An XPS spectrum of one region over 25 eV around the C1s peak. This illustrates the example in B.2.1.

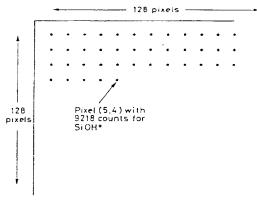


Figure A.2 - A SIMS map of one element setting the mass spectrometer to 45 amu. This illustrates the first block of the example in B.2.3.

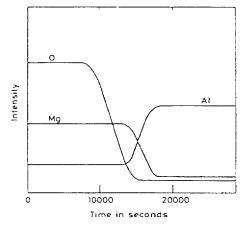


Figure A.3 - An AES cyclic sputter depth profile at one point with differential spectrum single values for each of three elements over 1000 depths lasting eight hours. This illustrates the example in B.2.6.

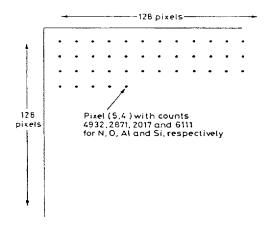


Figure A.4 - An AES map for four elements which may be transferred as one block. The data for the four elements may be transferred sequentially at each point, the counts for the elements being corresponding variables.

Annex A (informative)

Design of the format

Surface analysis provides the scientist with a wide range of techniques and many operating-parameters to vary. Usually the whole of the instrument, not just the spectrometer, is under computer control, allowing all the parameters to be automatically recorded. The complexity of the data-processing required for interpretation makes it essential to keep a complete record, and the transferred data should be equally complete. If all parameters are included in the format then each parameter can be identified by its position and the number of repetitions of a parameter can be indicated explicitly.

It is advantageous to use only those characters that appear on a normal display or printer since there is no difficulty in transferring these by communications protocols and manual checking of the data is possible. This is the principle upon which the design of the present Format is based⁽²⁾.

For data transfer it is envisaged that the procedure would be for the sending computer to write the formatted data to a text-file, for the text-file to be transferred to the receiving computer, and for the receiving computer to convert the data into its own data-structures, as three separate operations. The text-file could be transferred over a communications-link using a standard file-transfer protocol such as KERMIT, XMODEM or local area network protocol, or by writing it to a portable storage medium such as a floppy disk and exchanging the medium between compatible systems. The text-file could also be used as an intermediary between two incompatible programs running on the same computer. File-transfer details such as data-compression or error-checking are not specified in the format since these should be effected by the communications protocol. The present format simply defines the order in which the characters are to be assembled by the data-capture computer for transmission and in which they are expected to be received by the data-receiving computer.

The Format encompasses several kinds of experiment. The simplest experiment is a single spectrum of counts versus some regularly-scanned variable such as energy or mass, and the Format can encode this kind of data as an abscissa start, an abscissa increment and a list of ordinate values. The Format also covers a spectrum in which there is a complete set of single values of a fixed number of variables at each abscissa value. For rare cases in which there is no regularly-scanned variable the Format can encode data consisting of complete sets of corresponding values of two or more variables. These two scan modes are called REGULAR and IRREGULAR, respectively. A third scan mode, MAPPING, is used when the data are in the form of a map.

Any of the above types of spectrum can be encoded as a block of data, and provided that all have the same scan mode any number of such spectra can be assembled into a single overall experiment. Each spectrum may be obtained by any of the following techniques: AES diff (differentiated Auger electron spectroscopy), AES dir (direct Auger electron spectroscopy), EDX (energy dispersive X-ray spectroscopy), ELS (electron energy loss spectroscopy), FABMS (fast atom bombardment mass spectroscopy), ISS (ion scattering spectroscopy), SIMS (secondary ion mass spectroscopy), SNMS (sputtered neutral mass spectroscopy), UPS (ultra-violet photoelectron spectroscopy), XPS (X-ray photoelectron spectroscopy) and XRF (X-ray fluorescence spectroscopy). In the mass spectroscopies the spectrum is usually a function of mass but may instead be a function of the emitted particle energy at a given mass, and the corresponding techniques are distinguished as FABMS energy spec, SIMS energy spec and SNMS energy spec, respectively.

It is common in a surface analysis experiment for each spectrum to refer to a different point on the sample surface, as in a map, or to a different depth below the sample surface, as in sputter depth profiling. This kind of relationship between the spectra in an experiment is encoded by means of an experiment mode. Four of these experiment modes are MAP, SDP, MAPDP, and NORM. In MAP each spectrum refers to a specified point in a regular two-dimensional spatial array. In SDP each spectrum refers to a specified layer in a composition sputter depth profile. In MAPDP each spectrum refers to a specified point in a regular two-dimensional spatial array in a specified layer in a composition sputter depth profile. In NORM each spectrum may be independent of the others, or each spectrum may refer to a specified set of single values of one or more experimental variables such as temperature or time. NORM can also be used for data not in spectral form.

As a result of data-reduction in the data-capture computer, or because of the design of the experiment, instead of having spectra we may have a complete set of single values of a fixed number of variables for every point in a map or depth in a profile. In this case we can encode the map or profile as a single block instead of as a whole experiment. For this we include the four experiment modes MAPSV, SDPSV, SEM and MAPSVDP. In MAPSV each set of values refers to one point in a regular two-dimensional spatial array. In SDPSV each set of values refers to one layer in a composition depth profile. SEM is a map

of electron emission intensities. In MAPSVDP each set of values in a block refers to one point in a regular two-dimensional spatial array, and successive blocks refer to successive layers in a composition sputter depth profile. For a map, the block includes information on how the sets of values are to be arranged in rows and columns.

Very many kinds of experiment are covered by the above options. For instance, a linescan is a restricted case of MAPSV, and a multi-point depth profile with spectra may involve selecting only a few of the possible positions in MAPDP. The Format also covers non-standard applications such as spectrometer intensity/energy response functions and ratio scatter diagrams for AES and EDX.

In many experiments it is important to know the angles of incidence and emission of the various radiations. Here these angles are specified with respect to the fixed orthogonal coordinate system of the sample-stage x, y and z shift directions as shown in figure 1, rather than with respect to a coordinate system established with reference to the sample itself. Although angles referred to the sample itself would be more significant physically, only the fixed reference system is directly available to the data-capture computer. The angles of the sample may be deduced from settings of parameters of the instrument but the converse is not always true. The propagation of errors and the reduction of mistakes are both best effected by the recording of primary data rather than deduced data.

It may help to give the broad outline of the structure of the Format here. What is defined by the Format is an *experiment*. This consists of a set of parameters that apply to the experiment as a whole, followed by a number of *blocks*, followed by an experiment terminator. Each block consists of a set of parameters that apply only to that block, followed by a series of ordinate values representing a curve, spectrum or map. The parameters that apply to the experiment as a whole fall into the following groups in the order in which they appear:

identity of the experiment in its research environment optional comments experiment mode number of blocks and how they are arranged pointers to manually-entered parameters future-upgrade parameters.

The parameters that apply to a block fall into the following groups in the order in which they appear:

identity of the block in the experiment identity of the sample date and time optional comments technique analysis analyser spectral-recording sputtering sample orientation additional parameters and future-upgrade parameters

To illustrate the use of the Format a wide range of examples are given in Annex B. To aid the busy programmer who may be provided with no more than a very limited suite of options by his surface analysis instrument Annex C gives selected simple partially-encoded versions of the Format, derived from the Format of Clause 2, which may be used in certain traditional straightforward circumstances. This Format is based on the earlier VAMAS Standard Data Transfer Format⁽²⁾ but has three changes: (i) the spectrometer geometry description is based on a right handed rather than left handed co-ordinate system (ii) the number of entries in the parameter inclusion or exclusion list has been set to zero to simplify the format and (iii) the carriage return sequence has been changed from the single 7 bit ASCII character CARRIAGE RETURN to the two character sequence CARRIAGE RETURN followed by LINE FEED. The latter is the correct "end of line marker" in text files on a range of computer types. To assist programmers to decode this Format, skeleton programs are provided in reference (2). Note, however, that those programs can read and make use of a non-zero number of entries in the parameter inclusion or exclusion list, ie they can read both this and the original VAMAS Format. Additionally, those programs do not, of course, allow for item (iii) above.

Annex B (informative)

Examples of the format

B.1 General

Examples of the Format are given in B.2.1 to B.2.12. The items beginning an experiment, that is, from format identifier up to and including the comment lines, and the last item, that is, the experiment terminator, have been omitted in all cases. Similarly, the items beginning the blocks, namely block identifier, number of lines in block comment and the block comment lines have been omitted. The characters in the transferred text are shown indented, and to save space in printing here, carriage return is replaced by COMMA plus SPACE. Examples of items from institution identifier to experiment identifier could be NPL, VG ESCALAB 2, P J Cumpson, Mass Study; in the block the items years to number of hours in advance of Greenwich Mean Time would be 1986, 5, 1, 18, 45,21, 0. These are straightforward and so are not repeated.

B.2 Archetypal applications

Clause B.3 provides a detailed annotation of examples B.2.1 to B.2.4, respectively.

B.2.1 An XPS spectrum of one region over 25 eV around the C 1s peak.

The experiment parameters are as above plus

NORM, REGULAR, 1, 0, 0, 0, 0, 0, 1,

There is one block with parameters as above plus

XPS, Al. 1486.6, 300, 500, 500, 45, 90, FAT, 20, 3, 4.5, 0, 1000, 5000, 15, 0, C, 1s, -1, binding energy, eV, 275, 0.05, 1, counts per channel, d, pulse counting, 0.5, 1, 400E-9, 0, 0, 0, 501, 3214, 33008, followed by the 501 ordinate values.

B.2.2 An AES depth profile at one point with narrow-scan direct spectra of three elements, the first being oxygen.

The experiment parameters are

SDP, REGULAR, 3, 1, time in seconds, s, 0, 0, 0, 0, 300,

There are 300 blocks. The parameters of the first block are

AES dir, 0, electron gun, 18, 1, 1, 5000, 10, 3, 3, 45, 180, FRR, 4, 3, 4.5, 0, 2000, 5000, 15, 0, O, KLL, -1, kinetic energy, eV, 530, -0.5, 1, counts per channel, d, pulse counting, 0.5, 1, 400E-9, 2000, 120, 500, 500, 20, 270, continuous, 0, 0, 0, 0, 100, 20154, 31192,

followed by the 100 ordinate values.

B.2.3 Two SIMS maps of elements, setting the mass spectrometer to two discrete settings of mass, the first being 45 amu.

The experiment parameters are

MAPSV, MAPPING, 1, unified atomic mass units, u, 0, 0, 0, 0, 2,

There are two blocks. The parameters of the first block are

SIMS, 45, gallium gun, 31, 1, 1, 10000, 1.3, 0.1, 0.1, 12.8, 12.8, 1, 1, 128, 1, 128, 128, 20, 270, constant delta m, 0.9, 1, 4.3, 0, 12.8, 12.8, 0, 180, SiOH, 1, 1, 1, counts per pixel, d, pulse counting, 0.03, 1, 400E-9, 0, 0, 0, 0, 16384, 294, 681,

B.2.4 An AES depth profile of differential spectra of three elements, the first being oxygen, at four points on an integrated circuit.

This is an example where some positions in the map are left empty.

The experiment parameters are

MAPDP, REGULAR, 3, 4, 128, 128, 1, time in seconds, s, 0, 0, 0, 0, 1200,

There are 1200 blocks. The parameters of the first block are

AES diff, 15, 38, 0, electron gun, 18, 1, 1, 5000, 1020, 2, 2, 300, 300, 45, 180, FRR, 4, 5, 3, 4.5, 0, 2000, 5000,

16

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15, 0, O, KLL, -1, kinetic energy, eV, 530, -0.5, 1, counts per channel, d, analogue, 0.5, 1, 400E-9, 2000, 120, 500, 500, 20, 270, cyclic, 0, 0, 0, 100, 381, 4320, followed by the 100 ordinate values.

B.2.5 Five SNMS spectral regions of a stainless steel containing tin as a function of ten oxygen exposures.

The experiment parameters are

NORM, REGULAR, 5, 1, oxygen exposure in seconds, s, 0, 0, 0, 0, 50,

There are 50 blocks. The parameters of the first block are

SNMS, 0, argon, 18, 1, 1, 100, 10000, 3000, 3000, 0, 0, constant delta m, 0.9, 1, 5.1, 0, 1000, 1000, 30, 180, Sn, 0, 0, mass, u, 120.5, -0.1, 1, counts per channel, d, pulse counting, 0.03, 1, 400E-9, 0, 0, 0, 0, 31, 15, 38941, followed by the 31 ordinate values.

B.2.6 An AES cyclic sputter depth profile at one point with differential spectrum single values for each of three elements over 1000 depths lasting eight hours.

The experiment parameters are

SDPSV, REGULAR, 0, 0, 0, 0, 0, 1,

There is one block with parameters

AES diff, electron gun, 18, 1, 1, 5000, 1020, 100, 100, 45, 180, FRR, 4, 5, 3, 4.5, 0, 1000, 5000, 15, 0, AI Mg O, KLL, -1, time in seconds, s, 0, 28.8, 3, Al intensity, d, Mg intensity, d, O intensity, d, analogue, 3, 1, 400E-9, 2000, 120, 3000, 3000, 20, 270, cyclic, 0, 0, 0, 3000, 381, 4320, 23, 9793, 782, 5640,

followed by the 3000 ordinate values. Alternatively this could have been sent as three blocks corresponding to Al, Mg and O respectively. This would be equally valid.

B.2.7 SIMS Energy spectra 0 to 100 eV of three elements at five positions on an integrated circuit followed over 100 depths in a profile lasting one hour.

The spectral region, 0 to 100 eV, no longer defines the element uniquely so we use the experimental variables to do this.

The experiment parameters are

MAPDP, REGULAR, 1, 5, 128, 128, 2, unified atomic mass units, u, time in seconds, s, 0, 0, 0, 0, 1500,

There are 1500 blocks. The parameters of the first block are

SIMS energy spec, 37, 21, 28, 0, argon, 18, 1, 1, 1000, 100, 0.5, 0.5, 300, 300, 20, 270, constant delta m, 0.9, 1, 2.0, 0, 1E37, 1E37, 0, 0, Si, 1, 1, electron volts, eV, 0, 0.2, 1, counts per channel, d, pulse counting, 0.03, 1, 400E-9, 0, 0, 0, 0, 501, 0, 4927,

followed by the 501 ordinate values.

B.2.8 Combined AES spectra of three elements and one EDX spectrum for a full map as a function of sputtering depth at 100 depths.

The experiment parameters are

MAPDP, REGULAR, 4, 16384, 128, 128, 1, time in seconds, s, 0, 0, 0, 6553600,

There are 6553600 blocks! The parameters of the first block are

AES dir, 1, 1, 0, electron gun, 18, 1, 1, 20000, 25, 0.2, 0.2, 300, 300, 45, 180, FRR, 2, 3, 4, 5, 2000, 5000, 15, 0, O, KLL, -1, electron volts, eV, 520, -1, 1, counts per channel, d, pulse counting, 0.03, 1, 400E-9, 2000, 1020, 3000, 3000, 20, 270, cyclic, 0, 0, 0, 0, 31, 831, 5420,

followed by the 31 ordinate values.

B.2.9 AES x linescan of four elements at peak and background in the direct spectrum mode across an integrated circuit about 2/3 of way down screen.

The experiment parameters are

MAPSV, MAPPING, 1, kinetic energy eV, eV, 0, 0, 0, 0, 8,

There are eight blocks. The parameters of the first block are

AES dir, 530, electron gun, 5000, 10, 0.1, 0.1, 12.8, 12.8, 1, 40, 128, 40, 128, 40, 45, 180, FRR, 2, 3, 4.5, 0, 2000,

5000, 15, 0, O, KLL, -1, 1, counts per channel, d, pulse counting, 0.01, 1, 400E-9, 0, 0, 0, 0, 128, 3081, 34333, followed by the 128 ordinate values. Alternatively, we could use one block of eight corresponding variables followed by 1024 ordinate values. C.2.6 shows how the corresponding variable approach works.

B.2.10 A correction curve for scaling AES spectra.

The experiment parameters are

NORM, REGULAR, 1, 0, 0, 0, 0, 0, 1,

There is one block with parameters

AES dir, electron gun, 1E37, 1E37, 1E37, 1E37, 1E37, 1E37, FRR, 4, 3, 4.5, 0, 2000, 5000, 15, 0, all elements, any, -1, kinetic energy eV, eV, 0, 0.5, 1, normalising factor, d, pulse counting, 3, 1, 0, 0, 0, 0, 0, 4001, 0, 10000, followed by the 4001 ordinate values.

B.2.11 A sputter-depth profile following two SIMS intensities, target bias and sputtering-time at irregular intervals.

The experiment parameters are

SDPSV, IRREGULAR, 1, unified atomic mass units, u, 0, 0, 0, 0, 2,

There are two blocks. The parameters of the first block are

SIMS, 11, oxygen, 8, 2, 1, 5000, 900, 500, 500, 20, 270, constant delta m, 0.9, 1, 3.0, 1E37, 300, 300, 0, 0, boron, 1, 1, 3, counts per channel, d, target bias, V, sputtering time, s, pulse counting, 2, 1, 400E-9, 0, 0, 0, 0, 300, 2, 100517, -2.8, -1.7, 0, 3581,

followed by the 300 ordinate values.

B.2.12 A ratio scatter diagram in AES for 100 analyses of three elements.

The experiment parameters are

NORM, IRREGULAR, 0, 0, 0, 0, 0, 0, 1,

There is one block with parameters

AES dir, electron gun, 20000, 10, 0.01, 0.01, 45, 180, FAT, 50, 1, 4.5, 0, 2000, 5000, 15, 0, AI Mg Si, KLL, -1, 3, AI intensity (N1-N2)/(N1+N2), d, Mg intensity (N1-N2)/(N1+N2), d, Si intensity (N1-N2)/(N1+N2), d, pulse counting, 1, 1, 400E-9, 0, 0, 0, 0, 300, 0, 1, 0, 1, 0, 1,

followed by the 300 ordinate values.

B.3 Annotated examples

Dummy headings and some comments have been added, and the *format identifier* has been abbreviated to save space. Particular instrument and identifiers are given in the examples but these have no particular significance beyond illustrating the text of the entry.

B.3.1 Annotation of example in B.2.1

VAMAS Surface Chemical etc
NPL
Kratos XSAM 800
WAD
Gold medal contamination
1
example 1
NORM
REGULAR
1
0
0
0
0
0

and a of block	1
number of blocks	l las blook id
block identifier	1st block id
sample identifier	1st sample id
year in full	1986
month	5
day of month	1
hours	18
minutes	45
seconds	21
number of hours in advance of Greenwich Mean Time	0
number of lines in block comment	0
technique	XPS
analysis source label	Al
analysis source characteristic energy	1486.6
analysis source strength	300
analysis source beam width x	500
analysis source beam width y	500
analysis source polar angle of incidence	45
analysis source azimuth	90
analyser mode	FAT
analyser pass energy or retard ratio or mass resolution	20
magnification of analyser transfer lens	3
analyser work function or acceptance energy of atom or ion	
target bias	0
analysis width x	1000
analysis width y	5000
analyser axis take off polar angle	15
analyser axis take off azimuth	0
species label	C
transition or charge state label	1s
charge of detected particle	-1
abscissa label	binding energy
abscissa units	eV
abscissa start	275
abscissa increment	0.05
number of corresponding variables	1
corresponding variable label	counts per channel
corresponding variable units	d
signal mode	pulse counting
signal collection time	0.5
number of scans to compile this block	1
signal time correction	400E-9
sample normal polar angle of tilt	0
sample normal tilt azimuth	0
sample rotation angle	0
number of additional numerical parameters	0
number of ordinate values	501
minimum ordinate value	3214
maximum ordinate value	33008
followed by 501 ordinate values and	
experiment terminator	end of experiment

B.3.2 Annotation of example B.2.2

format identifier VAMAS Surface Chemical *etc* institution identifier NPL

```
Riber MAC 2
instrument model identifier
                                                            WAD
operator identifier
                                                            Tantalum pentoxide standard
experiment identifier
number of lines in comment
                                                            1
                                                            example 2
comment line
                                                            SDP
experiment mode
                                                            REGULAR
scan mode
number of spectral regions
number of experimental variables
                                                            1
experimental variable label
                                                            time in seconds
experimental variable units
                                                            0
                                                            0
number of manually entered items in block
                                                            0
number of future upgrade experiment entries
                                                            0
number of future upgrade block entries
                                                            300
number of blocks
                                                            1st block id
block identifier
sample identifier
                                                            1st sample id
year in full
                                                            1986
month
                                                            5
day of month
                                                            1
hours
                                                            18
minutes
                                                            45
                                                            21
seconds
number of hours in advance of Greenwich Mean Time
                                                            0
number of lines in block comment
                                                            0
                                                            AES dir
technique
value of experimental variable
                                                            0
analysis source label
                                                            electron gun
sputtering ion or atom atomic number
                                                            18
number of atoms in sputtering ion or atom particle
                                                            1
sputtering ion or atom charge sign and number
                                                            1
                                                            5000
analysis source characteristic energy
analysis source strength
                                                            10
analysis source beam width x
                                                            3
analysis source beam width y
                                                            3
analysis source polar angle of incidence
                                                            45
analysis source azimuth
                                                            180
analyser mode
                                                            FRR
analyser pass energy or retard ratio or mass resolution
                                                            4
magnification of analyser transfer lens
                                                            3
analyser work function or acceptance energy of atom or ion 4.5
target bias
analysis width x
                                                            2000
                                                            5000
analysis width y
analyser axis take off polar angle
                                                            15
analyser axis take off azimuth
                                                           0
species label
                                                           O
transition or charge state label
                                                           KLL
charge of detected particle
                                                           -1
abscissa label
                                                           kinetic energy
abscissa units
                                                           eV
abscissa start
                                                           530
                                                           -0.5
abscissa increment
number of corresponding variables
corresponding variable label
                                                           counts per channel
```

corresponding variable units signal mode pulse counting signal collection time 0.5 number of scans to compile this block 1 signal time correction 400E-9 sputtering source energy 2000 sputtering source beam current 120 sputtering source width x 500 sputtering source width y 500 sputtering source polar angle of incidence 20 sputtering source azimuth 270 sputtering mode continuous sample normal polar angle of tilt 0 sample normal tilt azimuth 0 sample rotation angle 0 number of additional numerical parameters 0 number of ordinate values 100 minimum ordinate value 20154 maximum ordinate value 31192 followed by 100 ordinate values, 299 more blocks and experiment terminator end of experiment

B.3.3 Annotation of example B.2.3

format identifier VAMAS Surface Chemical etc institution identifier **NPL** instrument model identifier VG SIMSLAB MIG 300 operator identifier WAD experiment identifier IC 4261 number of lines in comment comment line example experiment mode **MAPSV** scan mode MAPPING number of experimental variables experimental variable label unified atomic mass units experimental variable units 0 number of manually entered items in block 0 number of future upgrade experiment entries 0 number of future upgrade block entries n number of blocks 2 block identifier 1st block id sample identifier 1st sample id year in full 1986 month 5 day of month 1 hours 18 minutes 45 seconds 21 number of hours in advance of Greenwich Mean Time 0 number of lines in block comment 0 technique SIMS value of experimental variable 45 analysis source label gallium gun sputtering ion or atom atomic number 31 number of atoms in sputtering ion or atom particle 1

1

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sputtering ion or atom charge sign and number

```
10000
         analysis source characteristic energy
                                                                      1.3
         analysis source strength
         analysis source beam width x
                                                                      0.1
         analysis source beam width y
                                                                      0.1
                                                                      12.8
         field of view x
                                                                      12.8
         field of view y
                                                                      1
         first linescan start x coordinate
         first linescan start y coordinate
                                                                      1
         first linescan finish x coordinate
                                                                      128
         first linescan finish y coordinate
                                                                      1
                                                                      128
         last linescan finish x coordinate
                                                                      128
         last linescan finish y coordinate
                                                                      20
         analysis source polar angle of incidence
                                                                      270
         analysis source azimuth
                                                                      constant delta m
         analyser mode
                                                                      0.9
         analyser pass energy or retard ratio or mass resolution
         magnification of analyser transfer lens
                                                                      1
         analyser work function or acceptance energy of atom or ion 4.3
                                                                      0
         target bias
                                                                      12.8
         analysis width x
         analysis width y
                                                                      12.8
         analyser axis take off polar angle
         analyser axis take off azimuth
                                                                      180
                                                                      SiOH
         species label
         transition or charge state label
                                                                      1
                                                                      1
         charge of detected particle
         number of corresponding variables
                                                                      1
                                                                      counts per pixel
         corresponding variable label
        corresponding variable units
                                                                      pulse counting
         signal mode
         signal collection time
                                                                      0.03
         number of scans to compile this block
         signal time correction
                                                                      400E-9
         sample normal polar angle of tilt
                                                                      n
         sample normal tilt azimuth
                                                                      0
         sample rotation angle
                                                                      0
         number of additional numerical parameters
                                                                      0
        number of ordinate values
                                                                      16384
        minimum ordinate value
                                                                      294
                                                                      681
        maximum ordinate value
followed by 16384 ordinate values, the second block and
        experiment terminator
                                                                      end of experiment
        Annotation of example B.2.4
```

B.3.4

```
VAMAS Surface Chemical etc
format identifier
institution identifier
                                                         NPL
instrument model identifier
                                                         PHI Multiprobe 610
                                                         WAD
operator identifier
                                                         IC failure diagnoses
experiment identifier
number of lines in comment
comment line
                                                         example 4
experiment mode
                                                         MAPDP
scan mode
                                                         REGULAR
number of spectral regions
```

```
number of analysis positions
  number of discrete x coordinates available in full map
                                                               128
  number of discrete y coordinates available in full map
                                                               128
  number of experimental variables
                                                               1
  experimental variable label
                                                              time in seconds
  experimental variable units
                                                              0
 number of manually entered items in block
                                                              0
 number of future upgrade experiment entries
                                                              0
 number of future upgrade block entries
                                                              0
 number of blocks
                                                              1200
 block identifier
                                                              1st block id
 sample identifier
                                                              1st sample id
 year in full
                                                              1986
 month
                                                              5
 day of month
                                                              1
 hours
                                                              18
 minutes
                                                              45
 seconds
                                                              21
 number of hours in advance of Greenwich Mean Time
                                                              0
 number of lines in block comment
                                                              0
 technique
                                                              AES diff
 x coordinate
                                                              15
 y coordinate
                                                              38
 value of experimental variable
                                                             0
 analysis source label
                                                             electron gun
 sputtering ion or atom atomic number
                                                              18
 number of atoms in sputtering ion or atom particle
                                                              1
 sputtering ion or atom charge sign and number
 analysis source characteristic energy
                                                             5000
 analysis source strength
                                                             1020
analysis source beam width x
                                                             2
analysis source beam width y
                                                             2
field of view x
                                                             300
field of view y
                                                             300
analysis source polar angle of incidence
                                                             45
analysis source azimuth
                                                             180
analyser mode
                                                             FRR
analyser pass energy or retard ratio or mass resolution
                                                             4
differential width
                                                             5
magnification of analyser transfer lens
                                                             3
analyser work function or acceptance energy of atom or ion 4.5
target bias
analysis width x
                                                             2000
analysis width y
                                                             5000
analyser axis take off polar angle
                                                             15
analyser axis take off azimuth
                                                            O
species label
                                                            0
transition or charge state label
                                                            KLL
charge of detected particle
                                                            - 1
abscissa label
                                                            kinetic energy
abscissa units
                                                            eV
abscissa start
                                                            530
abscissa increment
                                                            -0.5
number of corresponding variables
                                                            1
corresponding variable label
                                                            counts per channel
```

corresponding variable units đ analogue signal mode signal collection time 0.5 number of scans to compile this block 1 400E-9 signal time correction 2000 sputtering source energy 120 sputtering source beam current 500 sputtering source width x sputtering source width y 500 sputtering source polar angle of incidence 20 sputtering source azimuth 270 cyclic sputtering mode sample normal polar angle of tilt 0 sample normal tilt azimuth 0 sample rotation angle 0 number of additional numerical parameters 0 number of ordinate values 100 minimum ordinate value 381 maximum ordinate value 4320 followed by 100 ordinate values, 1199 more blocks and experiment terminator end of experiment

24

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Annex C (informative)

Partially encoded versions of the format

C.1 General

A partially-encoded version of the Format may be more appropriate for users whose instruments only provide a limited range of options. In these versions constants replace the variables defining the kind of experiment, and parameters that the Format would automatically omit because of these values are omitted. In C.2 to C.4 are partially-encoded versions for three frequently-used kinds of experiment. It should be stressed that these versions produce exactly the same output as that produced by the Format in Clause 2 for the same kind of experiment; the only difference is in their range of applicability. These versions do not cover manually entered items.

C.2 An experiment involving a number of regularly-scanned spectra or spectral regions for one technique as a function of one experimental variable, the analysis not being at a specifically-addressed point on the sample.

The example from B.2.5 illustrates this.

```
experiment = format identifier,
                  institution identifier.
                  instrument model identifier.
                 operator identifier.
                 experiment identifier.
                 number of lines in comment.
                  comment line}
                          (* The number of occurrences of comment line is specified by the value of number of lines in
                          comment above.
                              The comment may include details of the last calibration of the instrument. *),
                  'NORM', carriage return,
                  'REGULAR', carriage return,
                 number of spectral regions,
                  '1', carriage return,
                 experimental variable label,
                 experimental variable units,
                  '0', carriage return,
                  '0', carriage return,
                  '0', carriage return,
                 '0', carriage return,
                 number of blocks,
                 (block) -
                          (* The minus-sign followed by the empty-sequence, that is, nothing but the separator, indicates that
                          there must be at least one block.
                            The number of occurrences of block is specified by the value of number of blocks above. *).
                 experiment terminator;
block
             block identifier
             sample identifier,
             year in full
                 (* Gregorian calendar year, for example, '1987' *),
             month,
             day of month,
             hours,
             minutes,
             seconds
                 (* If the value of any of the above six items is not known the value -1 should be entered as a dummy
             number of hours in advance of Greenwich Mean Time,
```

```
number of lines in block comment,
(comment line)
    (* The number of occurrences of comment line is specified by the value of number of lines in block comment
    above. *),
technique,
value of experimental variable
    (* value of experimental variable may be, for example, total time in seconds, total sputtering time in seconds,
    total sputtering fluence in ions per m<sup>2</sup>, temperature in Kelvin, energy in electron volts or mass in unified
    atomic mass units. Where this variable changes smoothly with time this value shall be the value at the start
    of recording the block data unless specified otherwise in the experimental variable label. *),
analysis source label,
[sputtering ion or atom atomic number,
number of atoms in sputtering ion or atom particle,
sputtering ion or atom charge sign and number]
    (* The above three entries are inserted if and only if the value of technique is 'FABMS', 'FABMS energy
    spec', 'SIMS', 'SIMS energy spec', 'SNMS', 'SNMS energy spec' or 'ISS'. *),
analysis source characteristic energy
    (* energy in electron volts *),
analysis source strength
    (* power in watts for XPS and XRF; beam current in nanoamps for AES, EDX, ISS, SIMS and SNMS;
    beam equivalent for FABMS *),
analysis source beam width x
    (* width in micrometres at the sample in the plane perpendicular to the source beam *),
analysis source beam width y
    (* width in micrometres at the sample in the plane perpendicular to the source beam *),
analysis source polar angle of incidence
    (* degrees from upward z-direction, defined by the sample stage *),
analysis source azimuth
    (* degrees clockwise from the y-direction, defined by the sample stage*),
analyser mode,
analyser pass energy or retard ratio or mass resolution
    (* energy in electron volts, mass in amu *),
[differential width]
    (* electron volts peak-to-peak for sinusoidal modulation or computer differentiation.
      differential width is inserted if and only if the value of technique is 'AES diff'. *),
magnification of analyser transfer lens,
analyser work function or acceptance energy of atom or ion
    (* positive value for work function in electron volts for AES, XPS, UPS, ELS and ISS. The acceptance
    energy of an ion is the energy filter pass energy of the mass spectrometer for SIMS, SNMS and FABMS.*),
target bias
    (* target bias is in volts, including the sign. *),
analysis width x
    (* The analysis width x is the gated signal width of the source in the x-direction in the plane perpendicular
    to the beam for FABMS, FABMS energy spec, ISS, SIMS, SIMS energy spec, SNMS and SNMS energy
    spec, the analyser slit length divided by the magnification of the analyser transfer lens to that slit for AES
    diff, AES dir, ELS, UPS and XPS, and is the source width in the x-direction for both EDX and XRF.
       analysis width x is in micrometres. *),
analysis width y
    (* As analysis width x but for y. *),
analyser axis take off polar angle
   (* degrees from upward z-direction, defined by the sample stage *),
analyser axis take off azimuth
   (* degrees clockwise from the y-direction, defined by the sample stage*),
species label
   (* elemental symbol or molecular formula *),
```

transition or charge state label

```
(* for example, 'KLL' for AES, '1s' for XPS, '-1' for SIMS *),
              charge of detected particle
                  (* for example, -1 for AES and XPS, +1 for positive SIMS *),
              abscissa label,
              abscissa units,
              abscissa start,
              abscissa increment,
              '1', carriage return,
              corresponding variable label
                  (* The corresponding variable will be intensity in this case *),
              corresponding variable units,
              signal mode,
              signal collection time
                  (* time in seconds per scan for each channel or array-point, except for both EDX and XRF where it is the
                  total spectrum collection time *),
              number of scans to compile this block,
              signal time correction
                  (* This is the system dead time, except for EDX and XRF where it is the livetime-corrected acquisition time.
                  In the case of a dead time, a positive value indicates that the count rate should be corrected by dividing by
                  (1 - measured rate x dead time) whereas a negative value indicates a correction by multiplying by (exp(true
                  count rate x dead time)). If the spectra have already been corrected for dead time the value here will be zero
                  and the value of the dead time used will be noted in a comment line or elsewhere.
                     signal time correction is in seconds. *),
              sample normal polar angle of tilt
                  (* degrees from upward z-direction, defined by the sample stage *),
              sample normal tilt azimuth
                 (* degrees clockwise from the y-direction, defined by the sample stage*),
              sample rotation angle
                 (* degrees clockwise rotation about the sample normal. If this is referenced to a particular direction on the
                 sample this direction would be specified in a block comment line. *),
             number of additional numerical parameters,
             (additional numerical parameter label,
             additional numerical parameter units,
             additional numerical parameter value)
                 (* The number of occurrences of the above group of three entries is specified by the value of number of
                 additional numerical parameters above. *),
             number of ordinate values,
             minimum ordinate value,
             maximum ordinate value,
             {ordinate value} -
                 (* The number of occurrences of ordinate value is specified by the value of number of ordinate values
                 above.*);
abscissa increment = real number
             (* For units see the table under abscissa start. *);
abscissa label = text line;
abscissa start = real number;
abscissa units = units
             (* The table below shows the usual values of abscissa units for values of technique as a guide but is not
             mandatory.
```

technique	units
AES diff, AES dir, EDX, ELS, ISS, UPS, XPS, XRF	'eV'
FABMS, SIMS, SNMS	'u' or 's'
FABMS energy spec, SIMS energy spec, SNMS energy spec	'eV'

*);

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```
additional numerical parameter label = text line;
additional numerical parameter units = units;
additional numerical parameter value = real number;
analyser axis take off azimuth = real number;
analyser axis take off polar angle = real number;
analyser mode = ('FAT' | 'FRR' | 'constant delta m' | 'constant m/delta m' ), carriage return;
analyser pass energy or retard ratio or mass resolution = real number;
analyser work function or acceptance energy of atom or ion = real number;
analysis source azimuth = real number;
analysis source beam width x = real number;
analysis source beam width y = real number;
analysis source characteristic energy = real number;
analysis source label = text line;
analysis source polar angle of incidence = real number;
analysis source strength = real number;
analysis width x = real number;
analysis width y = real number;
block identifier = text line;
carriage return = ? 7-bit ASCII character CARRIAGE RETURN followed by 7-bit ASCII character LINE FEED?;
               · ' | '!' | '"' | '#' | '$' | '%' | '&' | "'" | '(' | ')' | '*' | '+' | ',' | '-' | '.' | '/'
                                                                       1':' 1';'
                                                           1 '8' | '9'
             | '0' | '1' | '2' | '3' | '4' | '5' | '6' | '7'
              '@' | 'A' | 'B' | 'C' | 'D' | 'E' | 'F' | 'G' | 'H' | 'I' | 'J'
                                                                            | 'K' | 'L' | 'M' | 'N' | 'O'
                                                                                         | ']' | '^'
                  'Q' | 'R' | 'S' | 'T' | 'U' | 'V' | 'W' | 'X' | 'Y' | 'Z' | 'Y' | '\'
              P'
             | ''' | 'a' | 'b' | 'c' | 'd' | 'e' | 'f' | 'g' | 'h' | 'i' | 'j' | 'p' | 'q' | 'r' | 's' | 't' | 'u' | 'v' | 'w' | 'x' | 'y' | 'z'
                                                                            | 'k'
                                                                                        | 'm' | 'n'
                                                                                  | '1'
                                                                            1'(' | '|' | ')'
             (* A character is the character SPACE or any of the 94 graphic characters specified in the American National
             Standard for Information Systems - Coded character sets - 7-bit American national standard code for information
             interchange (7-Bit ASCII), ANSI X3.4-1986. 7-bit ASCII is the American national version of the International
             Standard - Information processing - ISO 7-bit coded character set for information interchange, ISO 646-1983.
             or '~'. *);
charge of detected particle = integer;
comment line = text line;
corresponding variable label = text line;
corresponding variable units = units;
day of month = integer;
decimal number = [sign], [ {digit}, '.' ], {digit} -
        (* The minus-sign followed by the empty-sequence indicates that there must be at least one digit in decimal
        number.*);
differential width = real number;
digit = '0' | '1' | '2' | '3' | '4' | '5' | '6' | '7' | '8' | '9';
experiment identifier = text line;
experiment terminator = 'end of experiment', carriage return;
experimental variable label = text line;
experimental variable units = units;
format identifier = 'VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4', carriage return;
hours = integer;
institution identifier = text line;
instrument model identifier = text line;
integer = [sign], [digit] -, carriage return
        (* The value of integer must be in the range -1E37 to 1E37. *);
magnification of analyser transfer lens = real number;
maximum ordinate value = real number:
minimum ordinate value = real number;
minutes = integer;
month = integer;
```

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```
number of additional numerical parameters = zero or more;
  number of atoms in sputtering ion or atom particle = one or more;
  number of blocks = one or more;
  number of hours in advance of Greenwich Mean Time = real number;
  number of lines in block comment = zero or more;
  number of lines in comment = zero or more;
  number of ordinate values = one or more;
  number of scans to compile this block = one or more;
  number of spectral regions = one or more;
 one or more = integer
          (* The value of one or more must be greater than zero. *);
 operator identifier = text line;
 ordinate value = real number:
 real number = decimal number, [ 'E', [sign], {digit} - ], carriage return
          (* The value of real number must be in the range -1E37 to -1E-37, or zero, or in the range 1E-37 to 1E37.
             The minus-sign followed by the empty-sequence indicates that the exponent part, if present, must contain at least
          one digit. *);
 sample identifier = text line;
 sample normal polar angle of tilt = real number;
 sample normal tilt azimuth = real number;
 sample rotation angle = real number;
 seconds = integer;
 sign = '+' | '-':
 signal collection time = real number;
 signal mode = ( 'analogue' | 'pulse counting' ), carriage return
         (* Analogue signals, while recorded digitally, may be of either sign and have a gain which may be noted in the block
         comment. Pulse counting signals are integers with values equal to or greater than zero. *);
 signal time correction = real number;
 species label = text line;
 sputtering ion or atom atomic number = one or more;
 sputtering ion or atom charge sign and number = integer;
 target bias = real number;
technique = ('AES diff' | 'AES dir' | 'EDX' | 'ELS' | 'FABMS' | 'FABMS energy spec' | 'ISS' | 'SIMS' | 'SIMS
         energy spec' | 'SNMS' | 'SNMS energy spec' | 'UPS' | 'XPS' | 'XRF' ), carriage return;
 text line = 80*[character], carriage return;
 transition or charge state label = text line;
units = ('c/s' | 'd' | 'degree' | 'eV' | 'K' | 'micro C' | 'micro m' | 'm/s' | 'n' | 'nA' | 'ps' | 's' | 'u' | 'V' ), carriage
           (* These values are abbreviations for the units listed below:
                                  counts per second
              'c/s'
              'ď'
                                  dimensionless - just a number, eg, counts per channel
              'degree'
                                  angle in degrees
              'eV'
                                  electron volts
              'K'
                                  Kelvin
             'micro C'
                                  microcoulombs
             'micro m'
                                  micrometres
             'm/s'
                                  metres per second
             'n
                                  not defined here - may be given in a label
             'nA'
                                  nanoamps
             'ps'
                                  picoseconds
             's'
                                  seconds
             'u'
                                  unified atomic mass units
                                  volts
value of experimental variable = real number;
year in full = integer;
```

zero or more = integer

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```
C.3 An experiment involving a number of regularly-scanned spectral regions as a function of sputtering as in a sputter
depth profile by one technique such as AES or SIMS, the analysis not being at a particularly addressed point on the
sample.
The example from B.2.2 illustrates this.
experiment = format identifier,
                institution identifier,
                instrument model identifier,
                operator identifier,
                experiment identifier,
                number of lines in comment,
                {comment line}
                          (* The number of occurrences of comment line is specified by the value of number of lines in
                          comment above.
                              The comment may include details of the last calibration of the instrument. *),
                'SDP', carriage return,
                'REGULAR', carriage return,
                number of spectral regions,
                '1', carriage return,
                'time in seconds', carriage return,
                's', carriage return,
                '0', carriage return,
                '0', carriage return,
                '0', carriage return,
                '0', carriage return,
                number of blocks,
                {block} -
                          (* The minus-sign followed by the empty-sequence, that is, nothing but the separator, indicates that
                          there must be at least one block.
                            The number of occurrences of block is specified by the value of number of blocks above. *),
                experiment terminator;
block
             block identifier.
             sample identifier,
             year in full
                (* Gregorian calendar year, for example, '1987' *),
             month,
             day of month,
             hours,
             minutes,
             seconds
                (* If the value of any of the above six items is not known the value -1 should be entered as a dummy value.
             number of hours in advance of Greenwich Mean Time,
             number of lines in block comment.
             {comment line}
                (* The number of occurrences of comment line is specified by the value of number of lines in block comment
                above. *),
             technique,
             value of experimental variable
                (* value of experimental variable may be, for example, total sputtering time in seconds at the start of recording
                each block *),
             analysis source label,
```

(* The value of zero or more must be equal to or greater than zero. *);

```
sputtering ion or atom atomic number,
      number of atoms in sputtering ion or atom particle,
      sputtering ion or atom charge sign and number,
      analysis source characteristic energy
        (* energy in electron volts *),
      analysis source strength
        (* power in watts for XPS and XRF; beam current in nanoamps for AES, EDX, ISS, SIMS and SNMS; beam
        equivalent for FABMS *),
      analysis source beam width x
        (* width in micrometres at the sample in the plane perpendicular to the source beam *),
      analysis source beam width y
        (* width in micrometres at the sample in the plane perpendicular to the source beam *),
      analysis source polar angle of incidence
        (* degrees from upward z-direction, defined by the sample stage *),
      analysis source azimuth
        (* degrees clockwise from the y-direction, defined by the sample stage *),
     analyser mode,
     analyser pass energy or retard ratio or mass resolution
        (* energy in electron volts, mass in amu *),
      [differential width]
        (* electron volts peak-to-peak for sinusoidal modulation or computer differentiation.
          differential width is inserted if and only if the value of technique is 'AES diff'. *),
     magnification of analyser transfer lens,
     analyser work function or acceptance energy of atom or ion
        (* positive value for work function in electron volts for AES, XPS, UPS, ELS and ISS. The acceptance
        energy of an ion is the energy filter pass energy of the mass spectrometer for SIMS, SNMS and FABMS, *).
     target bias
        (* target bias is in volts, including the sign. *),
     analysis width x
        (* The analysis width x is the gated signal width of the source in the x-direction in the plane perpendicular
        to the beam for FABMS, FABMS energy spec, ISS, SIMS, SIMS energy spec, SNMS and SNMS energy spec,
       the analyser slit length divided by the magnification of the analyser transfer lens to that slit for AES diff, AES
       dir, ELS, UPS and XPS, and is the source width in the x-direction for both EDX and XRF.
          analysis width x is in micrometres. *),
     analysis width y
       (* As analysis width x but for y. *),
     analyser axis take off polar angle
       (* degrees from upward z-direction, defined by the sample stage *),
     analyser axis take off azimuth
       (* degrees clockwise from the y-direction towards the operator, defined by the sample stage *),
     species label
       (* elemental symbol or molecular formula *),
     transition or charge state label
       (* for example, 'KLL' for AES, '1s' for XPS, '-1' for SIMS *),
    charge of detected particle
       (* for example, -1 for AES and XPS, +1 for positive SIMS *),
    abscissa label,
    abscissa units,
    abscissa start,
    abscissa increment,
    '1', carriage return,
corresponding variable label
       (* The corresponding variable will be intensity in this case *),
corresponding variable units,
signal mode,
signal collection time
```

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```
(* time in seconds per scan for each channel or array-point, except for both EDX and XRF where it is the total
                spectrum collection time *),
        number of scans to compile this block,
         signal time correction
                (* This is the system dead time, except for EDX and XRF where it is the livetime-corrected acquisition time.
                In the case of a dead time, a positive value indicates that the count rate should be corrected by dividing by
                (1 - measured rate x dead time) whereas a negative value indicates a correction by multiplying by (exp(true
                count rate x dead time)). If the spectra have already been corrected for dead time the value here will be zero
                and the value of the dead time used will be noted in a comment line elsewhere.
                  signal time correction is in seconds. *),
         sputtering source energy
                (* energy in electron volts *),
         sputtering source beam current
                (* current in nanoamps or equivalent for neutrals *),
        sputtering source width x
                (* width in micrometres at the sample in the plane perpendicular to the sputtering source beam *),
         sputtering source width y
                (* width in micrometres at the sample in the plane perpendicular to the sputtering source beam *),
        sputtering source polar angle of incidence
                (* degrees from upward z-direction, defined by the sample stage *),
         sputtering source azimuth
                (* degrees clockwise from the y-direction, defined by the sample stage *),
         sputtering mode)
                (* The value of sputtering mode is either 'continuous', when sputtering continues while spectral data is being
                recorded, or 'cyclic', when sputtering is suspended while spectral data is being recorded.
                The above seven entries are for a sputtering source used in addition to the analysis source, as in depth
                profiling, in AES diff, AES dir, EDX, ELS, UPS, XPS or XRF.
                  The above seven entries are inserted if and only if the value of technique is 'AES diff', 'AES dir', 'EDX',
                'ELS', 'UPS', 'XPS' or 'XRF'. *),
        sample normal polar angle of tilt
                (* degrees from upward z-direction, defined by the sample stage *),
        sample normal tilt azimuth
                (* degrees clockwise from the y-direction towards the operator, defined by the sample stage *),
        sample rotation angle
                (* degrees clockwise rotation about the sample normal. If this is referenced to a particular direction on the
                sample this direction would be specified in a block comment line. *),
        number of additional numerical parameters,
         {additional numerical parameter label,
        additional numerical parameter units,
        additional numerical parameter value)
                (* The number of occurrences of the above group of three entries is specified by the value of number of
                additional numerical parameters above. *),
        number of ordinate values.
        minimum ordinate value.
        maximum ordinate value.
         {ordinate value} -
                (* The number of occurrences of ordinate value is specified by the value of number of ordinate values
                above.*);
abscissa increment = real number
        (* For units see the table under abscissa start. *);
abscissa label = text line;
abscissa start = real number;
abscissa units = units
        (* The table below shows the usual values of abscissa units for values of technique as a guide but is not mandatory.
```

technique	units
AES diff, AES dir, EDX, ELS, ISS, UPS, XPS, XRF	'eV'
FABMS, SIMS, SNMS	'u' or 's'
FABMS energy spec, SIMS energy spec, SNMS energy spec	'eV'

```
additional numerical parameter label = text line;
 additional numerical parameter units = units;
 additional numerical parameter value = real number;
 analyser axis take off azimuth = real number;
 analyser axis take off polar angle = real number;
 analyser mode = ('FAT' | 'FRR' | 'constant delta m' | 'constant m/delta m' ), carriage return;
 analyser pass energy or retard ratio or mass resolution = real number;
 analyser work function or acceptance energy of atom or ion = real number;
 analysis source azimuth = real number;
 analysis source beam width x = real number;
 analysis source beam width y = real number:
 analysis source characteristic energy = real number:
 analysis source label = text line;
 analysis source polar angle of incidence = real number;
 analysis source strength = real number;
 analysis width x = real number;
 analysis width y = real number,
 block identifier = text line;
 carriage return = ? 7-bit ASCII character CARRIAGE RETURN followed by 7-bit ASCII character LINE FEED?;
                      1 .i. | ....
                                 | '#' | '$' | '%' | '&' | """ | '(' | ')' | '*'
 character =
                                                                               1'+'1',
                ,0, |,1,
                            1 '2' |
                                  '3'
                                       '4'
                                                        1 '7'
                                             1 '5'
                                                   6'
                                                               | '8' | '9'
                 '@' | 'A' | 'B' | 'C'
                                      | 'D'
                                             | 'E'
                                                  'F'
                                                         'G'
                                                              | 'H' | 'I'
                                                                               | 'K' | 'L' | 'M' | 'N' | 'O'
                                                                           ٠J،
                 'P' | 'Q' | 'R' | 'S'
                                       'T' | 'U' | 'V'
                                                        'W' | 'X' | 'Y' | 'Z' | '\
                                                                                           1 ']' | '^'
                     | 'a' | 'b' | 'c' | 'd'
                                            | 'e' | 'f' | 'g' | 'h' | 'i' | 'j' | 'k' | 'I' | 'u' | 'v' | 'w' | 'x' | 'y' | 'z' | '{' | '| '
                                                                                          'm' | 'n'
                l'p' |'q' |'r' |'s'
                                      't'
                                                                                          | '}'
             (* A character is the character SPACE or any of the 94 graphic characters specified in the American National
             Standard for Information Systems - Coded character sets - 7-bit American national standard code for information
             interchange (7-Bit ASCII), ANSI X3.4-1986. 7-bit ASCII is the American national version of the International
             Standard - Information processing - ISO 7-bit coded character set for information interchange, ISO 646-1983.
             or '~', *);
charge of detected particle = integer;
comment line = text line;
corresponding variable label = text line;
corresponding variable units = units;
day of month = integer;
decimal number = [sign], [ {digit}, '.' ], {digit} -
        (* The minus-sign followed by the empty-sequence indicates that there must be at least one digit in decimal
        number.*);
differential width = real number;
digit = '0' | '1' | '2' | '3' | '4' | '5' | '6' | '7' | '8' | '9';
experiment identifier = text line;
experiment terminator = 'end of experiment', carriage return;
format identifier = 'VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4', carriage return;
hours = integer;
institution identifier = text line;
instrument model identifier = text line;
```

@ ISO

ISO 14976:1998(E)

```
integer = [sign], {digit} - , carriage return
         (* The value of integer must be in the range -1E37 to 1E37. *);
magnification of analyser transfer lens = real number;
maximum ordinate value = real number;
minimum ordinate value = real number;
minutes = integer;
month = integer;
number of additional numerical parameters = zero or more;
number of atoms in sputtering ion or atom particle = one or more;
number of blocks = one or more:
number of hours in advance of Greenwich Mean Time = real number;
number of lines in block comment = zero or more;
number of lines in comment = zero or more;
number of ordinate values = one or more;
number of scans to compile this block = one or more;
number of spectral regions = one or more;
one or more = integer
        (* The value of one or more must be greater than zero. *);
operator identifier = text line:
ordinate value = real number;
real number = decimal number, { 'E', [sign], {digit} - ], carriage return
        (* The value of real number must be in the range -1E37 to -1E-37, or zero, or in the range 1E-37 to 1E37.
            The minus-sign followed by the empty-sequence indicates that the exponent part, if present, must contain at least
        one digit. *);
sample identifier = text line;
sample normal polar angle of tilt = real number;
sample normal tilt azimuth = real number;
sample rotation angle = real number;
seconds = integer;
sign = '+' | '-';
signal collection time = real number;
signal mode = ('analogue' | 'pulse counting'), carriage return
        (* Analogue signals, while recorded digitally, may be of either sign and have a gain which may be noted in the block
        comment. Pulse counting signals are integers with values equal to or greater than zero. *);
signal time correction = real number;
species label = text line;
sputtering ion or atom atomic number = one or more;
sputtering ion or atom charge sign and number = integer;
sputtering mode = ('continuous' | 'cyclic'), carriage return;
sputtering source azimuth = real number;
sputtering source beam current = real number;
sputtering source energy = real number;
sputtering source polar angle of incidence = real number;
sputtering source width x = real number;
sputtering source width y = real number;
target bias = real number;
technique = ( 'AES diff' | 'AES dir' | 'EDX' | 'ELS' | 'FABMS' | 'FABMS energy spec' | 'ISS' | 'SIMS' | 'SIMS energy spec' | 'SNMS' | 'SNMS energy spec' | 'UPS' | 'XPS' | 'XRF' ), carriage return;
text line = 80*[character], carriage return;
transition or charge state label = text line;
units = ('c/s' | 'd' | 'degree' | 'eV' | 'K' | 'micro C' | 'micro m' | 'm/s' | 'n' | 'nA' | 'ps' | 's' | 'u' | 'V' ), carriage
        return
        (* These are abbreviations for
             'c/s'
                                  counts per second
              'd'
                                  dimensionless - just a number, eg, counts per channel
              'degree'
                                  angle in degrees
```

```
'eV'
                                   electron volts
              'K'
                                   Kelvin
              'micro C'
                                   microcoulombs
              'micro m'
                                   micrometres
              'm/s'
                                   metres per second
              'n
                                   not defined here - may be given in a label
              'nA'
                                   nanoamps
              'ps'
                                   picoseconds
              's'
                                   seconds
              'u'
                                  unified atomic mass units
             'V'
                                  volts
         *);
value of experimental variable = real number;
year in full = integer;
zero or more = integer
        (* The value of zero or more must be equal to or greater than zero. *);
C.4
        An experiment involving a number of maps of single values representing the intensities of different elements
        for one technique such as AES, EDX or SIMS, the maps to be made of x-linescans starting at (1,1) and varying
        with one experimental variable.
The example from B.2.3 illustrates this.
experiment =
                format identifier.
                 institution identifier,
                 instrument model identifier,
                 operator identifier,
                 experiment identifier,
                 number of lines in comment,
                 {comment line}
                         (* The number of occurrences of comment line is specified by the value of number of lines in
                         comment above.
                         The comment may include details of the last calibration of the instrument. *),
                 'MAPSV', carriage return,
                 'MAPPING', carriage return,
                 '1', carriage return,
                experimental variable label,
```

experimental variable units,

'0', carriage return,

'0', carriage return,

'0', carriage return,

'0', carriage return,

number of blocks,

{block} -

(* The minus-sign followed by the empty-sequence, that is, nothing but the separator, indicates that there must be at least one block.

The number of occurrences of block is specified by the value of number of blocks above. *), experiment terminator;

block = block identifier,

sample identifier,

year in full

(* Gregorian calendar year, for example, '1987' *),

month,

day of month,

hours,

minutes,

seconds

(* If the value of any of the above six items is not known the value -1 should be entered as a dummy value.*),

number of hours in advance of Greenwich Mean Time,

number of lines in block comment,

{comment line}

(* The number of occurrences of comment line is specified by the value of number of lines in block comment above. *),

technique,

value of experimental variable

(*value of experimental variable may be, for example, total time in seconds, total sputtering time in seconds, total sputtering fluence in ions per m², temperature in Kelvin, energy in electron volts or mass in unified atomic mass units. Where this variable changes smoothly with time this value shall be the value at the start of recording the block data unless specified otherwise in the experimental variable lablel*),

analysis source label,

[sputtering ion or atom atomic number,

number of atoms in sputtering ion or atom particle,

sputtering ion or atom charge sign and number]

(* The above three entries are inserted if and only if the value of technique is 'FABMS', 'FABMS energy spec', 'SIMS', 'SIMS energy spec', 'SNMS', 'SNMS energy spec' or 'ISS'. *),

analysis source characteristic energy

(* energy in electron volts *),

analysis source strength

(* power in watts for XPS and XRF; beam current in nanoamps for AES, EDX, ISS, SIMS and SNMS; beam equivalent for FABMS *),

analysis source beam width x

(* width in micrometres at the sample in the plane perpendicular to the source beam *), analysis source beam width y

(* width in micrometres at the sample in the plane perpendicular to the source beam *),

field of view x

(* micrometres *),

field of view y

(* micrometres *),

'1', carriage return,

'1', carriage return,

first linescan finish x coordinate,

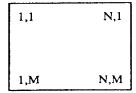
'1', carriage return,

last linescan finish x coordinate,

last linescan finish y coordinate

(* The above six entries are required for specifying the size and shape of the map and for relating the order in the scan sequence to the position on the sample.

In the coordinate system to be used, x-values start at unity at the left-hand side of the frame and increase towards the right-hand side, and y-values start at unity at the top of the frame and increase towards the bottom of the frame, as shown below.



*),

analysis source polar angle of incidence

(* degrees from upward z-direction, defined by the sample stage *),

```
analysis source azimuth
     (* degrees clockwise from the y-direction, defined by the sample stage *),
 analyser mode,
 analyser pass energy or retard ratio or mass resolution
     (* energy in electron volts, mass in amu *),
 [differential width]
     (* electron volts peak-to-peak for sinusoidal modulation or computer differentiation.
       differential width is inserted if and only if the value of technique is 'AES diff'. *),
 magnification of analyser transfer lens,
 analyser work function or acceptance energy of atom or ion
     (* positive value for work function in electron volts for AES, XPS, UPS, ELS and ISS. The acceptance
     energy of an ion is the energy filter pass energy of the mass spectrometer for SIMS, SNMS and FABMS.*),
 target bias
     (* target bias is in volts, including the sign. *),
 analysis width x
     (* The analysis width x is the gated signal width of the source in the x-direction in the plane perpendicular
     to the beam for FABMS, FABMS energy spec, ISS, SIMS, SIMS energy spec, SNMS and SNMS energy
     spec, the analyser slit length divided by the magnification of the analyser transfer lens to that slit for AES
     diff, AES dir, ELS, UPS and XPS, and is the source width in the x-direction for both EDX and XRF.
       analysis width x is in micrometres. *),
analysis width y
    (* As analysis width x but for y. *),
analyser axis take off polar angle
    (* degrees from upward z-direction, defined by the sample stage *),
analyser axis take off azimuth
    (* degrees clockwise from the y-direction, defined by the sample stage *),
species label
    (* elemental symbol or molecular formula *),
transition or charge state label
    (* for example, 'KLL' for AES, '1s' for XPS, '-1' for SIMS *),
charge of detected particle
    (* for example, -1 for AES and XPS, +1 for positive SIMS *),
number of corresponding variables
    (* If the data is in the form of sets of corresponding values of two or more variables then number of
    corresponding variables is set to the number of variables, otherwise it is set to unity. *),
{corresponding variable label,
corresponding variable units)
    (* The number of occurrences of the above pair of items is specified by the value of number of
    corresponding variables above. *),
signal mode,
signal collection time
    (* time in seconds per scan for each channel or array-point, except for both EDX and XRF where it is the
    total spectrum collection time *),
number of scans to compile this block,
signal time correction
    (* This is the system dead time, except for EDX and XRF where it is the livetime-corrected acquisition time.
    In the case of a dead time, a positive value indicates that the count rate should be corrected by dividing by
    (1 - measured rate x dead time) whereas a negative value indicates a correction by multiplying by (exp(true
    count rate x dead time)). If the spectra have already been corrected for dead time the value here will be zero
    and the value of the dead time used will be noted in a comment line or elsewhere.
      signal time correction is in seconds. *),
sample normal polar angle of tilt
    (* degrees from upward z-direction, defined by the sample stage *),
    (* degrees clockwise from the y-direction, defined by the sample stage *),
sample rotation angle
```

(* degrees clockwise rotation about the sample normal. If this is referenced to a particular direction on the

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```
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```

```
sample this direction would be specified in a block comment line. *),
             number of additional numerical parameters,
             {additional numerical parameter label,
             additional numerical parameter units,
             additional numerical parameter value)
                 (* The number of occurrences of the above group of three entries is specified by the value of number of
                 additional numerical parameters above. *),
             number of ordinate values
                 (* The value of number of ordinate values is equal to product of the value of number of corresponding
                 variables and the number of sets of corresponding variables to be transferred. *),
             minimum ordinate value,
             maximum ordinate value,
             (ordinate value) -
                 (* The number of occurrences of ordinate value is specified by the value of number of ordinate values
                 above.*);
additional numerical parameter label = text line;
additional numerical parameter units = units;
additional numerical parameter value = real number;
analyser axis take off azimuth = real number;
analyser axis take off polar angle = real number;
analyser mode = ( 'FAT' | 'FRR' | 'constant delta m' | 'constant m/delta m' ), carriage return;
analyser pass energy or retard ratio or mass resolution = real number;
analyser work function or acceptance energy of atom or ion = real number;
analysis source azimuth = real number;
analysis source beam width x = real number;
analysis source beam width y = real number;
analysis source characteristic energy = real number;
analysis source label = text line;
analysis source polar angle of incidence = real number;
analysis source strength = real number;
analysis width x = real number;
analysis width y = real number, block identifier = text line;
carriage return = ? 7-bit ASCII character CARRIAGE RETURN followed by 7-bit ASCII character LINE FEED ?;
               ''' | '!' | '''' | '#' | '$' | '%' | '&' | "''' | '(' | ')' | '*' | '+' | ','
character =
             | '0' | '1' | '2' | '3' | '4' | '5' | '6' | '7' | '8' | '9' | ':' | ';' | '<' | '=' | '>'
             '@' | 'A' | 'B' | 'C' | 'D' | 'E' | 'F' | 'G' | 'H' | 'I' | 'I' | 'K' | 'L' | 'M' | 'N' | 'O'
             | 'P' | 'Q' | 'R' | 'S' | 'T' | 'U' | 'V' | 'W' | 'X' | 'Y' | 'Z' | 'Y' | '\' ' | '\' ' | '\' ' ' ' ' '
             | ''' | 'a' | 'b' | 'c' | 'd' | 'e' | 'f' | 'g' | 'h' | 'i' | 'j' | 'k' | 'l' | 'm' | 'n'
             | 'p' | 'q' | 'r' | 's' | 't' | 'u' | 'v' | 'w' | 'x' | 'y' | 'z' | '(' | '|' | ')' | '-'
          (* A character is the character SPACE or any of the 94 graphic characters specified in the American National
          Standard for Information Systems - Coded Character Sets - 7-Bit American National Standard Code for Information
          Interchange (7-Bit ASCII), ANSI X3.4-1986. 7-Bit ASCII is the American national version of the International
          Standard Information processing - ISO 7-bit coded character set for information interchange, ISO 646-1983. Other
          charge of detected particle = integer;
comment line = text line;
corresponding variable label = text line;
corresponding variable units = units;
day of month = integer;
decimal number = [sign], [ (digit), '.' ], {digit} -
            (* The minus-sign followed by the empty-sequence indicates that there must be at least one digit in decimal
            number. *);
differential width = real number;
digit = '0' | '1' | '2' | '3' | '4' | '5' | '6' | '7' | '8' | '9';
```

```
experiment identifier = text line;
 experiment terminator = 'end of experiment', carriage return;
 experimental variable label = text line;
 experimental variable units = units:
 field of view x = real number;
 field of view y = real number;
 first linescan finish x coordinate = integer;
 format identifier = 'VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4', carriage return;
 hours = integer;
 institution identifier = text line;
 instrument model identifier = text line:
 integer = [sign], (digit) -, carriage return
              (* The value of integer must be in the range -1E37 to 1E37. *);
 last linescan finish x coordinate = integer;
 last linescan finish y coordinate = integer;
 magnification of analyser transfer lens = real number;
 maximum ordinate value = real number;
 minimum ordinate value = real number.
 minutes = integer;
 month = integer:
 number of additional numerical parameters = zero or more;
 number of atoms in sputtering ion or atom particle = one or more;
 number of blocks = one or more;
 number of corresponding variables = one or more;
 number of hours in advance of Greenwich Mean Time = real number;
number of lines in block comment = zero or more;
number of lines in comment = zero or more;
number of ordinate values = one or more;
number of scans to compile this block = one or more;
one or more = integer
              (* The value of one or more must be greater than zero. *);
operator identifier = text line;
ordinate value = real number;
real number = decimal number, [ 'E', [sign], {digit} - ], carriage return
             (* The value of real number must be in the range -1E37 to -1E-37, or zero, or in the range 1E-37 to 1E37.
                 The minus-sign followed by the empty-sequence indicates that the exponent part, if present, must contain at
             least one digit. *);
sample identifier = text line;
sample normal polar angle of tilt = real number;
sample normal tilt azimuth = real number;
sample rotation angle = real number;
seconds = integer;
sign = '+' | '-';
signal collection time = real number;
signal mode = ( 'analogue' | 'pulse counting' ), carriage return
             (* Analogue signals, while recorded digitally, may be of either sign and have a gain which may be noted in the
             block comment. Pulse counting signals are integers with values equal to or greater than zero. *);
signal time correction = real number;
species label = text line;
sputtering ion or atom atomic number = one or more;
sputtering ion or atom charge sign and number = integer;
target bias = real number;
technique = ( 'AES diff' | 'AES dir' | 'EDX' | 'ELS' | 'FABMS' | 'FABMS energy spec' | 'ISS' | 'SIMS' | 'SIMS
        energy spec' | 'SNMS' | 'SNMS energy spec' | 'UPS' | 'XPS' | 'XRF' ), carriage return;
text line = 80*[character], carriage return;
transition or charge state label = text line;
```

```
units = ('c/s' | 'd' | 'degree' | 'eV' | 'K' | 'micro C' | 'micro m' | 'm/s' | 'n' | 'nA' | 'ps' | 's' | 'u' | 'V' ), carriage
        (* These values are abbreviations for the units listed below:
             'c/s'
                                   counts per second
                                  dimensionless - just a number, eg, counts per channel
             'd'
                                   angle in degrees
             'degree'
             'eV'
                                   electron volts
                                   Kelvin
             'K'
                                   microcoulombs
             'micro C'
                                   micrometres
             'micro m'
                                   metres per second
             'm/s'
                                   not defined here - may be given in a label
             'n
             'nA'
                                   nanoamps
                                   picoseconds
             'ps'
             's'
                                   seconds
                                   unified atomic mass units
             'n
             v,
                                   volts
        *);
value of experimental variable = real number;
year in full = integer;
zero or more = integer
          (* The value of zero or more must be equal to or greater than zero. *);
```

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Annex D (informative)

Bibliography

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