Designation: E 2077 – 00

Standard Specification for Analytical Data Interchange Protocol for Mass Spectrometric Data[1]

This standard is issued under the fixed designation E 2077; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This specification covers a standardized format for mass spectrometric data representation and a software vehicle to effect the transfer of mass spectrometric data between instrument data systems. This specification provides a protocol designed to benefit users of analytical instruments and increase laboratory productivity and efficiency.

1.2 The protocol in this specification provides a standardized format for the creation of raw data files, library spectrum files or results files. This standard format has the extension ".cdf" (derived from NetCDF). The contents of the file include typical header information like instrument, sample, and acquisition method description, followed by raw, library or processed data. Once data have been written or converted to this protocol, they can be read and processed by software packages that support the protocol.

1.3 This specification does not provide for the storage of data acquired simultaneous to and integrated with the mass spectrometric data, but on other detectors; for example attached to the mass spectrometer's liquid or gas chromatographic system. Related Specification E 1947 and Guide 1948 describe the storage of 2-dimensional chromatographic data.

1.4 The software transfer vehicle used for the protocol in this specification is NetCDF, which was developed by the Unidata Program and is funded by the Division of Atmospheric Sciences of the National Science Foundation.[2]

1.5 The protocol in this specification is intended to (*1*) transfer data between various vendors' instrument systems, (*2*) provide Laboratory Information Management Systems (LIMS) communications, (*3*) link data to document processing applications, (*4*) link data to spreadsheet applications, and (*5*) archive analytical data, or a combination thereof. The protocol is a consistent, vendor independent data format that facilitates the analytical data interchange for these activities.

1.6 The protocol consists of:

1.6.1 This specification on mass spectrometric data, which gives the full definitions for each one of the generic mass spectrometric data elements used in implementation of the protocol. It defines the analytical information categories, which are a convenient way for sorting analytical data elements to make them easier to standardize.

1.6.2 Guide E 2078 on mass spectrometric data, which gives the full details on how to implement the content of the protocol using the public-domain NetCDF data interchange system. It includes a brief introduction to using NetCDF and describes an API (Application Programming Interface) that is intended to be incorporated into application programs to read or write NetCDF files. It is intended for software implementors, not those wanting to understand the definitions of data in a mass spectrometric dataset.

1.6.3 NetCDF Users Guide.

2. Referenced Documents

2.1 *ASTM Standards:*

E 2078 Guide for Analytical Data Interchange Protocol for Mass Spectrometric Data[3]

E 1443 Terminology Relating to Building and Accessing Materials and Chemical Databases[4]

E 1947 Specification for Analytical Data Interchange Protocol for Chromatographic Data[3]

E 1948 Guide for Analytical Data Interchange Protocol for Chromatographic Data[3]

2.2 *Other Standards:*

NetCDF User's Guide [5]

Occupational Safety and Health Administration (OSHA) Standards-29 CFR part 1910 [6]

IEEE 488 [7]

IEEE -802 [7]

EIA - 232 [8]

2.3 *ISO Standards:*[9]

[1] This specification is under the jurisdiction of ASTM Committee E13 on Molecular Spectroscopy and Chromatography and is the direct responsibility of Subcommittee E13.15 on Analytical Data.

Current edition approved March 10, 2000. Published July 2000.

[2] For more information on the NetCDF standard, contact Unidata at www.unidata.ucar.edu.

[3] *Annual Book of ASTM Standards*, Vol 03.06.

[4] *Annual Book of ASTM Standards*, Vol 14.01.

[5] Available from Russell K. Rew, Unidata Program Center, University Corporation for Atmospheric Research, P.O. Box 3000, Boulder, CO 80307-3000.

[6] Occupational Safety and Health Administration, U.S. Department of Labor.

[7] Institute of Electrical and Electronics Engineers, Inc., 445 Hoes Lane, P.O. Box 1331, Piscataway, NJ 08855–1331.

[8] Electronics Industries Alliance, 2500 WIlson Blvd., Arlington, VA 22201.

[9] Available from ISO, 1 Rue de Varembe, Case Postale 56, CH 1211, Geneve, Switzerland.

8601:1988 Data elements and interchange formats (First edition published 1988-06-15; with Technical Corrigendum 1 published 1991-05-01)

639: 1988 Code for the representation of names of languages

9000 Quality Management Systems

ISO/IEC - 8802

3. Terminology

3.1 *Analytical Information Classes*—The Mass Spectrometry Information Model categorizes mass spectrometric information into a number of information "classes." There is not a direct mapping of these classes into the implementation categories described further below. The implementation categories describe the information hierarchy; the classes describe the contents within the hierarchy. The model presented here only partially addresses these classes. In particular, the last two (Processed Results and Component Quantitation Results) are not described at all. Only Implementation Category 1 is required for compliance within this specification. Information about the other implementation categories is provided for historical interest. The classes defined here are:

3.1.1 *Administrative*—information for administrative tracking of experiments.

3.1.2 *Instrument-ID*—information about the instrument that generally does not change from experiment to experiment.

3.1.3 *Sample Description*—information describing the sample and its history, handling and processing.

3.1.4 *Test Method*—all information used to generate the raw data and processed results. This includes instrument control, detection, calibration, data processing and quantitation methods.

3.1.5 *Raw Data*—the data as stored in the data file, along with any parameters needed to describe it.

3.1.6 *Processed Results*—processing information and values derived from the raw data.

3.1.7 *Component Quantitation Results*—individual quantitation results for components in a complex mixture.

3.2 *Definitions for Administrative Information Class*—These definitions are for those data elements that are implemented in the protocol. See Table 1.

TABLE 1 Administrative Information Class

NOTE 1—Particular analytical information categories (C1, C2, C3, C4, or C5) are assigned to each data element under the Category column. The meaning of this category assignment is explained in Section 5.

NOTE 2—The Required column indicates whether a data element is required, and if required, for which categories. For example, M1234 indicates that that particular data element is required for any dataset that includes information from Category 1, 2, 3, or 4. M4 indicates that a data element is only required for Category 4 datasets.

NOTE 3—Unless otherwise specified, data elements are generally recorded to be their actual test values, instead of the nominal values that were used at the initiation of a test.

NOTE 4—A table is not to be interpreted as a table of keywords. The software implementation is independent of the data element names used here, and is in fact quite different. Likewise, the datatypes given are not an implementation representation, but a description of the form of the data element name. That is, a data element labeled as floating point may, for example, be implemented as a double precision floating point number; in this document, it is sufficient to note it as floating point without reference to precision.

Data Element Name	Datatype	Category	Required
dataset-completeness	string	C1	M12345
protocol-template-revision	string	C1	M12345
netcdf-revision	string	C1	M12345
languages	string	C1 or C5	. . .
administrative-comments	string	C1 or C2	. . .
dataset-origin	string	C1	M4
dataset-owner	string	C1	. . .
dataset-date-time-stamp	string	C1	M1234
injection-date-time-stamp	string	C1	M1234
experiment-title	string	C1	. . .
experiment-cross-references	string array[n]	C3 or C4	
operator-name	string	C1	M4
experiment-type	string	C1 or C4	. . .
pre-experiment-program-name	string	C2 or C5	. . .
post-experiment-program-name	string	C2 or C5	. . .
number-of-times-processed	integer	C5	
number-of-times-calibrated	integer	C5	
calibration-history	string array[n]	C5	
source-file-reference	string	C5	M4
source-file-format	string	C5	
source-file-date-time-stamp	string	C5	M4
external-file-references	string array[n]	C5	
error-log	string	C5	

3.2.1 *administrative-comments*—comments about the dataset identification of the experiment. This free text field is for anything in this information class that is not covered by the other data elements in this class.

3.2.2 *calibration-history*—an audit trail of file names and data sets which records the calibration history; used for Good Laboratory Practice (GLP) compliance.

3.2.3 *dataset-completeness*—indicates which analytical information categories are contained in the dataset. The string should exactly list the category values, as appropriate, as one or more of the following "C1+C2+C3+C4+C5," in a string separated by plus (+) signs. This data element is used to check for completeness of the analytical dataset being transferred.

3.2.4 *dataset-date-time-stamp*—indicates the absolute time of dataset creation relative to Greenwich Mean Time. Expressed as the synthetic datetime given in the form: YYYYMMDDhhmmss±ffff.

3.2.4.1 *Discussion*—This is a synthesis of ISO 8601, which compensates for local time variations.

3.2.4.2 *Discussion*—The YYYYMMDDhhmmss expresses the local time, and time differential factor (ffff) expresses the hours and minutes between local time and the Coordinated Universal Time (UTC or Greenwich Mean Time, as disseminated by time signals), as defined in ISO 8601. The time differential factor (ffff) is represented by a four-digit number preceded by a plus (+) or a minus (−) sign, indicating the number of hours and minutes that local time differs from the UTC. Local times vary throughout the world from UTC by as much as −1200 h (west of the Greenwich Meridian) and by as much as +1300 h (east of the Greenwich Meridian). When the time differential factor equals zero, this indicates a zero hour, zero minute, and zero second difference from Greenwich Mean Time.

3.2.4.3 *Discussion*—An example of a value for a datetime would be: 1991,08,01,12:30:23-0500 or 19910801123023-0500. In human terms this is 23 s past 12:30 PM on August 1, 1991 in New York City. Note that the −0500 h is 5 full hours time behind Greenwich Mean Time. The ISO standard permits the use of separators as shown, if they are required to facilitate human understanding. However, separators are not required and consequently shall not be used to separate date and time for interchange among data processing systems.

3.2.4.4 *Discussion*—The numerical value for the month of the year is used, because this eliminates problems with the different month abbreviations used in different human languages.

3.2.5 *dataset-origin*—name of the organization, address, telephone number, electronic mail nodes, and names of individual contributors, including operator(s), and any other information as appropriate. This is where the dataset originated.

3.2.6 *dataset-owner*—name of the owner of a proprietary dataset. The person or organization named here is responsible for this field's accuracy. Copyrighted data should be indicated here.

3.2.7 *error-log*—information that serves as a log for failures of any type, such as instrument control, data acquisition, data processing or others.

3.2.8 *experiment-cross-references*—an array of strings which reference other related experiments.

3.2.9 *experiment-title*—user-readable, meaningful name for the experiment or test that is given by the scientist.

3.2.10 *experiment-type*—name of the type of data stored in this file. Select one of the types in the following list.

3.2.10.1 *Discussion*—The valid types are:

centroided mass spectrum—a data set containing centroided single or multiple scan mass spectra. This includes selected ion monitoring/recording (SIM/SIR) data, represented as mass-intensity pairs. This is the default.

continuum mass spectrum—a data set containing single or multiple scan mass spectra in continuum (non-centroided or profile) form. Scans are represented as mass-intensity pairs, whether incrementally spaced or not.

library mass spectrum—a data set consisting of one or more spectra derived from a spectral library. This is distinguished from an experimental mass spectral data set in that each spectrum in the library set has associated chemical identification and other information.

3.2.10.2 *Discussion*—A required Raw Data Information parameter, the number of scans, is used to define the shape of the data in the file, that is, to differentiate between single and multiple spectrum files. Another parameter, the scan number, is used to determine whether multiple scan files have an order or relatedness between scans.

3.2.10.3 *Discussion*—Some instruments are capable of mixed mode data acquisition, for example, alternating positive/negative EI (Electron Ionisation) or CI (Chemical Ionisation) scans. In order to keep this interchange standard as simple as possible, **each scan mode must be treated as a separate data set** regardless of how the data are actually stored in the source data file. Alternating positive/negative EI data, for example, will generate *two* interchange files (possibly simultaneously, depending on the implementation); one for the positive EI scans and one for the negative EI scans. These files may be made mutually cross-referential using their "external-file-references" fields.

3.2.11 *external-file-references*—an array of strings listing file names referred to from within the raw data file. These could include, for example, tune parameter, method, calibration, reference, sequence, or other files. NetCDF files produced in parallel (such as paired files containing alternating EI/CI scans) should be cross-referenced here.

3.2.12 *injection-date-time-stamp*—indicates the absolute time of sample injection relative to Greenwich Mean Time. Expressed as the synthetic datetime given in the form: YYYYMMDDhhmmss ±ffff. See *dataset-date-time-stamp* for details of the ISO standard definition of a date-time-stamp.

3.2.13 *languages*—optional list of natural (human) languages and programming languages delineated for processing by language tools.

3.2.13.1 *ISO-639-language*—indicates a language symbol and country code from Annex B and D of the ISO-639 Standard.

3.2.13.2 *other-language*—indicates the languages and dialect using a user-readable name; applies only for those languages and dialects not covered by ISO 639 (such as programming language).

3.2.14 *netcdf-revision*—current revision level of the NetCDF data interchange system software being used for data transfer.

3.2.15 *number-of-times-calibrated—also for GLP compliance*, a count of the number of times the data were calibrated before yielding the final results.

3.2.16 *number-of-times-processed—for GLP compliance*, a count of the number of times the data were processed to yield the final results recorded in this file. An audit trail of the file names of previous processing must be provided.

3.2.17 *operator-name*—name of the person who ran the equipment, which acquired the current dataset.

3.2.18 *post-experiment-program-name*—name(s) of any program(s) used to process raw data after acquisition.

3.2.19 *pre-experiment-program name*—name(s) of any program(s) run prior to the start of acquisition.

3.2.20 *protocol-template-revision*—revision level of the template being used by implementers. This needs to be included to tell users which revision of E 2077 should be referenced for the exact definitions of terms and data elements used in a particular dataset; for example "1.0."

3.2.21 *source-file-date-time-stamp*—the date and time at which the source file was created. This has the same format as described above for the "experiment-date-time-stamp" field.

3.2.22 *source-file-format*—a string which describes the format of the data file used to produce the interchange file, for example: "HP ChemStation," "VG Opus I," "Finnigan INCOS," etc.

3.2.23 *source-file-reference*—adequate information to locate the original dataset. This information makes the dataset self-referenced for easier viewing and provides internal documentation for GLP-compliant systems.

3.2.23.1 *Discussion*—This data element should include the complete filename, including node name of the computer system. For UNIX this should include the full path name. For VAX/VMS this should include the node-name, device-name, directory-name, and file-name. The version number of the file (if applicable) should also be included. For personal computer networks this needs to be the server name and directory path.

3.2.23.2 *Discussion*—If the source file was a library file, this data element should contain the library name and serial number of the dataset.

3.3 *Definitions for Instrument-ID Information Class*—This class contains the generally experiment-independent information describing the instrument(s) on which the experiment was performed. Because each subcomponent of an instrument may require separate identification, the "instrument-component-. . ." data element names in Table 2 should be interpreted as occurring once for each identified component. Not all data element names may be relevant for each component.

TABLE 2 Instrument ID Information Class

Data Element Name	Datatype	Category	Required
instrument-component-number	integer	C5	M5
instrument-component-name	string	C5	M5
instrument-component-id	string	C5	M5
instrument-component-manufacturer	string	C4 or C5	M5
instrument-component-model-number	string	C4 or C5	M5
instrument-component-serial-number	string	C5	M5
instrument-component-id-comments	string	C5	M5
instrument-component-software-version	string	C2 or C5	M5
instrument-component-firmware-version	string	C2 or C5	M5
operating-system-revision	string	C5	M5
application-software-revision	string	C5	M5

3.3.1 *application-software-revision*—the name, revision level, and (optionally, if different from the component manufacturer) manufacturer of each software module (if any) used in acquisition and processing of the data by the data system. This data element name applies only to data system instrument components. Required for GLP compliance.

3.3.2 *instrument-component-firmware-version*—the revision level of the instrument component firmware (if any) when the data were acquired. This data element name applies only to non-data system instrument components. This becomes an Implementation Category 2 field when the revision level affects the data acquisition, processing, or results. An example might be the revision level of a read-only memory (ROM) chip contained on an imbedded controller board.

3.3.3 *instrument-component-id*—the laboratory's identification code for the instrument component; this might be an internal inventory control number.

3.3.4 *instrument-component-id-comments*—any free-form comments not covered in one of the other fields.

3.3.5 *instrument-component-manufacturer*—the name of the manufacturer of the instrument component. Version 1.0 does not specify an enumerated list; vendor implementations of the specification are expected to standardize on a convention.

3.3.6 *instrument-component-model-number*—the model number or name, or both, used by the manufacturer to identify the instrument component.

3.3.7 *instrument-component-name*—the generic descriptive name of the instrument component. Version 1.0 does not specify an enumerated list of component names, but a future version may. For example: "gas chromatograph," "data system," "GC column," "MS core."

3.3.8 *instrument-component-number*—provides an index number for the particular instrument component being identified. Note that the total number of instrument components is implicit, and therefore instrument components must be sequentially numbered, beginning with zero.

3.3.9 *instrument-component-serial-number*—the manufacturer's serial number, if any, for the instrument component.

3.3.10 *instrument-component-software-version*—the revision level of the instrument component software (if any) when the data were acquired. This data element name applies only to non-data system instrument components. This becomes an Implementation Category 2 field when the revision level affects the data acquisition, processing, or results. An example might be a software program for chromatograph run control downloaded from a host data system.

3.3.11 *operating-system-revision*—the name and revision level of the data system's operating system software (if any) when the data were acquired and processed. This data element name applies only to data system instrument components, of

which there might be more than one for hyphenated instruments. Required for GLP compliance.

3.4 *Definition for Sample Description Information Class*—This class contains mostly comment-style information concerning the sample itself, and is intended to be used for minimal GLP compliance. As this standard matures, more explicit chemical method information may be included here. See Table 3.

TABLE 3 Sample-Description Information Class

Date Element Name	Datatype	Category	Required
Sample-owner	string	C5	
sample-receipt-date-time-stamp	string	C5	
internal-sample-id	string	C1	
external-sample-id	string	C5	
sampling-procedure-name	string	C5	
Sample-preparation-procedure	string	C4	
Sample-state	string	C4	
Sample-matrix	string	C4	
Sample-storage-information	string	C5	
Sample-disposal-information	string	C5	
Sample-history	string	C5	
Sample-preparation-comments	string	C5	
Sample-id-comments	string	C5	
manual-handling-precautions	string	C5	

3.4.1 *external-sample-id*—the number or code assigned to the sample by the submitter or submitter's organization.

3.4.2 *internal-sample-id*—the number or code used to identify the sample within the mass spectrometry laboratory or in a LIMS used by the laboratory.

3.4.3 *manual-handling-precautions*—any safety issues which are of concern when the sample is manually handled.

3.4.3.1 *Discussion*—A future version of this interchange specification, which deals more fully with GLP, will likely be expanded to address other sample management issues.

3.4.4 *sample-disposal-information*—a description of the disposal procedure for the sample (also in accord with the United States Department of Labor Occupational Safety and Health Administration (OSHA) regulations).

3.4.5 *sample-history*—a description of the history of this particular sample, including any special handling, treatments, etc. to distinguish it from others from the same batch.

3.4.6 *sample-id-comments*—any comments not covered elsewhere. This might include laboratory notebook references, etc.

3.4.7 *sample-matrix*—a string describing the natural matrix from which the sample was selected. In a future revision, this field will be made an enumerated set.

3.4.8 *sample-owner*—the name of the sample owner or submitter. This may be different from the data set owner.

3.4.9 *sample-preparation-comments*—any comments concerning preparation not covered in other fields.

3.4.10 *sample-preparation-procedure*—a textual description of the procedure used to prepare the sample for analysis.

3.4.11 *sampling-procedure-name*—the name of the procedure used to select a sample from its natural (bulk) matrix. For example: "supercritical fluid extraction." This will be made a formal set of choices in a future revision.

3.4.12 *sample-receipt-date-time-stamp*—the date and time the sample was received in the laboratory or submitted for analysis. The ISO 8601 format is used for this field. This date and time is usually earlier than the data set date/time stamp, and may be important when analysis of a sample must occur within a specified period after receipt.

3.4.13 *sample-state*—a string field, specified as one of these choices:

Sample State

solid
liquid
gas
supercritical fluid
plasma
other state

3.4.14 *sample-storage-information*—a description of the storage conditions for the sample, which includes the storage location. This is for OSHA compliance.

3.5 *Definitions for Test Method Information Class*—This class contains the information required to reconstruct the sampling and acquisition of the raw data once the sample has been prepared for analysis. See Table 4.

NOTE 1—None of these data elements are required to be present in the file; where the data element is important to the interpretation of the raw data but is not present, a default value is assumed. The default value for a data element is given in **boldface** type where it is defined.

TABLE 4 Test Method Information Class

Data Element Name	Datatype	Category	Required
separation-experiment-type	string	C1	
mass-spectrometer-inlet	string	C1	
mass-spectrometer-inlet-temperature	float	C1	
ionization-mode	string	C1	
ionization-polarity	string	C1	
electron-energy	float	C1	
laser-wavelength	float	C1	
reagent-gas	string	C1	
reagent-gas-pressure	float	C1	
FAB-type	string	C1	
FAB-matrix	string	C1	
source-temperature	float	C1	
filament-current	float	C1	
emission-current	float	C1	
accelerating-potential	float	C1	
detector-type	string	C1	
detector-potential	float	C1	
detector-entrance-potential	float	C1	
resolution-type	string	C1	
resolution-method	string	C1	
scan-function	string	C1	
scan-direction	string	C1	
scan-law	string	C1	
scan-time	float	C1	
mass-calibration-file-name	string	C1	
external-reference-file-name	string	C1	
instrument-reference-file-name	string	C1	
instrument-parameter-comments	string	C1	

3.5.1 *accelerating-potential*—this field specifies the accelerating potential in volts.

3.5.2 *detector-entrance-potential—for detectors in which it is appropriate*, this field specifies the (signed) potential at the entrance to the detector relative to system ground, in volts.

3.5.3 *detector-potential—for detectors in which it is appropriate*, this field specifies the (signed) potential across the detector, in volts. Examples include electron multipliers and conversion dynodes.

3.5.4 *detector-type*—this specifies the detection method used, and is chosen from the following set.

Detector Type

electron multiplier
photomultiplier
Focal plane array
faraday cup
conversion dynode electron multiplier
conversion dynode photomultiplier
multi-collector
other detector

3.5.5 *electron-energy*—this field is relevant for electron impact ionization mode, and contains the electron energy in volts.

3.5.6 *emission-current*—this field gives the filament emission current in microamps. This is also relevant principally for EI and CI ionization.

3.5.7 *external-reference-file-name*—this field specifies the name of an external file which contains the reference spectrum of the material used as an external mass calibrant.

3.5.8 *FAB-matrix*—this field specifies the fast atom bombardment (FAB) matrix used, if any, for the FAB experiment type.

3.5.9 *FAB-type*—this field is relevant for fast atom bombardment, and specifies the atom or neutral used in the bombardment gun.

3.5.10 *filament-current*—this field gives the filament input current in amps. This is primarily relevant for EI and CI ionization modes.

3.5.11 *instrument-parameter-comments*—this is a catch-all field; it might contain instrument tuning parameters, vacuum system pressures, or any other parameter which might be of use in reconstructing the acquisition which is not covered above. As this specification is made more GLP-compliant in later versions, additional formal fields may be defined which contain information on such instrument parameters.

3.5.12 *internal-reference-file-name*—this field specifies the name of an external file which contains the reference spectrum of the material used as an internal calibrant.

3.5.13 *ionization-mode*—this field describes the technique used to ionize the sample. It is also a string, chosen from the following set. **Only one ionization mode is supported per interchange file**.

Ionization Method

electron impact
chemical ionization
fast atom bombardment
field desorption
field ionization
electrospray ionization
thermospray ionization
atmospheric pressure chemical ionization
plasma desorption
laser desorption
spark ionization
thermal ionization
other ionization

3.5.14 *ionization-polarity*—this field describes the polarity of the detected ions and is chosen from the set that follows. **Only one ionization polarity is supported per interchange file**.

Ionization Polarity

positive
negative

3.5.15 *laser-wavelength*—this field is relevant for laser desorption ionization, and contains the laser wavelength in nanometers.

3.5.16 *mass-calibration-file-name*—this field gives the name of the external file which contains the voltage to mass, time to mass, or other mass calibration data.

3.5.17 *mass-spectrometer-inlet*—this field describes the sample introduction interface. It has a string value, from the set:

Mass Spectrometer Inlet

membrane separator
capillary direct
open split
jet separator
direct inlet probe
septum
particle beam
reservoir
moving belt
atmospheric pressure chemical ionization
flow injection analysis
electrospray inlet
infusion
thermospray inlet
other probe inlet
other inlet

Electrospray includes ion spray, and is used to describe both the inlet as well as the ionization technique.

3.5.18 *mass-spectrometer-inlet-temperature*—this field specifies the temperature of the spectrometer inlet, if appropriate, in degrees centigrade.

3.5.19 *reagent-gas*—this field is relevant for chemical ionization mode, and specifies the CI reagent gas.

3.5.20 *reagent-gas-pressure—in CI mode*, this specifies the pressure of the CI reagent gas. Units will be agreed upon as part of the implementation.

3.5.21 *resolution-method*—specifies the method for determining spectrometer resolution. For example: “10 % peak valley,” “50 % peak height,” “90 % peak height.”

3.5.22 *resolution-type*—this field specifies the type of instrument resolution: constant over the mass range or proportional to mass. It is chosen from the set that follows. See the description of *resolution*, in the *Raw Data Per-Scan Information* section, (3.8) that follows.

Resolution Type

constant
proportional

3.5.23 *scan-direction*—this field specifies the direction in which the mass range was scanned during acquisition and is chosen from the following set. **It is not necessarily the same direction in which masses are recorded in the interchange file. Masses are always recorded in ascending order in the interchange file**.

Scan Direction

up
down