



Standard Specification for Analytical Data Interchange Protocol for Mass Spectrometric Data¹

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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 simultaneously 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 E1947 and Guide E1948 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 E2078 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*:³

E1947 Specification for Analytical Data Interchange Protocol for Chromatographic Data

E1948 Guide for Analytical Data Interchange Protocol for Chromatographic Data

E2078 Guide for Analytical Data Interchange Protocol for Mass Spectrometric Data

2.2 *Other Standards*:

EIA 232⁴

IEEE 488⁵

IEEE 802⁵

Occupational Safety and Health Administration (OSHA)

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

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

³ For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard’s Document Summary page on the ASTM website.

⁴ Available from Electronic Industries Alliance (EIA), 2500 Wilson Blvd., Arlington, VA 22201.

⁵ Available from Institute of Electrical and Electronics Engineers, Inc. (IEEE), 445 Hoes Ln., Piscataway, NJ 08854-4141, <http://www.ieee.org>.