Designation: E 1948 – 98 (Reapproved 2004)

Standard Guide for Analytical Data Interchange Protocol for Chromatographic Data[1]

This standard is issued under the fixed designation E 1948; 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 guide covers the implementation of the Chromatographic Data Protocol in analytical software applications. Implementation of this protocol requires:

1.1.1 Specification E 1947, which contains the full set of data definitions. The chromatographic data protocol is not based upon any specific implementation; it is designed to be independent of any particular implementation, so that implementations can change as technology evolves. The protocol is implemented in stages, to speed its acceptance through actual use.

1.1.2 Specification E 1947 contains a full description of the contents of the data communications protocol, including the analytical information categories with data elements and their attributes for most aspects of chromatographic tests.

1.2 The Analytical Information Categories are a practical convenience for breaking down the standardization process into smaller, more manageable pieces. It is easier for developers to build consensus and produce working systems based on smaller information sets, without the burden and complexity of the hundreds of data elements contained in all the categories. The categories also assist vendors and end users in using the guide in their computing environments.

1.3 The NetCDF Data Interchange System is the container used to communicate data between applications in a way that is independent of both computer architectures and end-user applications. In essence, it is a special type of application designed for data interchange.

1.4 The Common Data Language (CDL) Template for Chromatography is a language specification of the chromatography dataset being interchanged. With the use of the NetCDF utilities, this human-readable template can be used to generate an equivalent binary file and the software subroutine calls needed for input and output of data in analytical applications.

2. Referenced Documents

2.1 *ASTM Standards:* [2]

E 1947 Specification for Analytical Data Interchange Protocal for Chromatographic Data

2.2 *Other Standard:*

NetCDF User's Guide[3]

3. Features of the Chromatographic Data Interchange Implementation Guide

3.1 The chromatographic data protocol consists of: (*1*) the data contents (what is being transferred), and (*2*) the data container (how it is being transferred).

3.2 *Analytical Information Categories*—To make the standardization process more manageable, five Analytical Information Categories were defined:

1. Raw Data
2. Final Results
3. Full Data Processing Method
4. Full Chemical Method
5. Good Laboratory Practices Information

3.2.1 This guide covers implementation of Raw Data (Category 1) and Final Results (Category 2). The development committee has completed implementation and testing of information in these categories.

3.3 *Chromatography Data Elements*—Each data element specifies a piece of information that is to be stored or transferred to another system. A data element has a name, a definition, and may have some default attributes, such as its datatype, the analytical information category to which it belongs, and whether it is mandatory or recommended. A data element may also reference other data elements.

3.4 *NetCDF Data Interchange System*—NetCDF is a data interchange system designed specifically for the requirements of scientific data. It was developed to meet the requirements of

[1] This specification is under the jurisdiction of ASTM CommitteeE01 on Analytical Chemistry for Metals, Ores and Related Materials and is the direct responsibility of Subcommittee E01.25 on Laboratory Data Interchange and Information Management.

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[2] 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.

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

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