EMSA/MAS Standard Format for Spectral Data Exchange

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One of the frustrating problems experimentalists often encounter with computer based spectroscopic instrumentation is the general incompatibility of the data files recorded on different analysis systems. The rapid growth of inexpensive personal computers has resulted in an information explosion which has increased the desirability and need for a simple method for exchange of experimental data between scientists who may be office neighbors or transoceanic collaborators. While it is not reasonable to expect a particular manufacturers software, which was designed and optimized for specific hardware, to function on an competitor's system, it would be of enormous value to the microanalysis community to have a simple method for data interchange. This would allow, for example, the routine distribution of experimental data between research laboratories with a minimum of difficulty or would enable test spectra to be transported between data acquisition systems to compare different data analysis routines. These points as well as all the other merits of a standardized data format have been detailed elsewhere [1-4].

Independent of the manufacturers, several analysts have devised computer programs to translate data files between the various microanalysis system formats, however, in general, each program implements a scheme which is based upon the programmer's own needs and applications. It would be more efficient to have the instrument manufacturers adopt a standard protocol which would accomplish this goal. Unfortunately, this is unlikely to occur without guidance and direction from the user community. It is important to realize that a standard for data exchange would not preclude existing or future development of optimized data storage formats tailored to a specific set of hardware/software systems. Rather, the protocol should be considered as an option, which allows the user to translate selected data sets to a simple well defined format, which can be subsequently transmitted (electronically or otherwise) to colleagues. Agreeing upon a format is, of course, a major obstacle. The minimum information necessary would, besides the actual spectrum include narrative text to describe the file, as well as all relevant calibration constants and instrument operating parameters needed to reconstruct the spectrum and to quantitatively analyze the data. The format should be as simple as possible, such that a file if necessary can be simply printed and still present valuable information to the analyst. Thus, storage as simple printable characters, rather than the more efficient binary mode, would appear to be the most desirable format. Based upon these general arguments, we believe that a standard format must possess the following attributes:

1. The format must be simple and easy to use.
2. The format must be both human and machine (i.e. computer) readable.
3. It must not be tied to any specific computer, programming language or operating system.
4. It must be capable of exactly presenting the data without loss of scientific content.

5. By recording all relevant instrumental parameters and experimental conditions, each file must contain enough information to uniquely identify the type and origin of the spectral data, to reconstruct its significance, and perform quantitative analysis if so desired .
6. It must be usable with all existing electronic communication networks (such as Bitnet,Internet...), telecommunications equipment (modems, Faxes) and all storage media (disks, tapes, hardcopy print..)
7. The format must support all spectra of interest to the microanalysis community (XEDS, EELS, AES, etc.) and be flexible enough to service future data sets, not yet specified.
8. Where possible, the format should be compatible with various commercial data plotting or analysis programs (i.e. spreadsheets, or graphical packages).
9. The proposed format need not be the most efficient storage mechanism. Its primary goals, as stated above, will generally prevent storage efficiency, which is the logical role of the host system file format, not the exchange format. If anything this format will err on the side of simplicity and ease of use.

The format employed by the Electron Microscopy and Microanalysis Public Domain Library (EMMPDL) [1,5] has the virtue of simplicity for XEDS and EELS, but is considered too rigid for more general use. The format proposed by a previous EMSA/MAS Task Force [3,4] addresses many problems but maybe too complicated for everyday use. The VMAS format [6] is also too complex for our perceived purpose, while the JCAMP-DX format, used by the infrared spectroscopy[2] is specific and detailed but is not appropriate to the interests of the EM community. The format proposed by this Task Force, which is too lengthy to document here, is a combination of what we perceive to be the best features of all the above formats, but is less complicated and has features tailored to the major EM Spectroscopies. A demonstration, discussion and detailed description of the format will be presented and distributed at the the 1991 EMSA/MAS meeting. Details will be published in the EMSA Bulletin [7] and are available through the EMMPDL[1]. The companion problem of a standard format for digital image storage is sufficiently different to warrant its own standard and will be a subject of future discussion. For the present, the TIFF (Vers. 5.0) format appears suitable for simple image storage. Spectrum-Image files, however, present a different problem and may need to be addressed by an appropriate Task Force.

REFERENCES

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