

JCAMP-DX for Electron Magnetic Resonance (IUPAC Recommendations 2006)

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The Joint Committee on Atomic and Molecular Physical data-Data eXchange (JCAMP-DX) is an evolving, open-ended, machine-independent, self-documenting file format for exchanging and archiving data from computerized laboratory instruments such as spectrometers and diffractometers whose output is commonly represented as spectral (profile) plots, contours, or peak tables. The first JCAMP-DX protocol was designed to meet the need for exchanging infrared spectra between similar instruments of different manufacturers. The present document is the result of ongoing efforts by users and manufacturers to extend JCAMP-DX to other types of instrumental data.

A major objective of JCAMP-DX is to enable routine capture of data at the source to make it available for exchange, archiving, and entry into databases. All data are represented as labeled fields of variable length using printable ASCII characters. A JCAMP-DX file is a text file that can be viewed, corrected, and annotated with ASCII text editors. Use of the name JCAMP-DX in the description of software capability implies the ability to generate and read JCAMP-DX files as defined in the relevant published protocols for a particular datatype.

This version of JCAMP-DX provides for a description of the file structure to be used to accommodate a very wide range of electron magnetic resonance applications. As much as it is very desirable for instrument data systems to be able to read and write files in a standard format directly, instrument vendors are encouraged to develop JCAMP-DX software for the instruments they currently support. This standard of the JCAMP-DX was further extended to cover Y2K-compatible date strings and good laboratory practice, and the next release will cover the information needed for storing n-dimensional data sets.



www.iupac.org/publications/pac/2006/7803/7803x0613.html

Uncertainty Estimation and Figures of Merit for Multivariate Calibration (IUPAC Technical Report)

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This report gives an introduction to multivariate calibration from a chemometrics perspective and reviews the various proposals to generalize the well-established univariate methodology to the multivariate domain. Univariate calibration leads to relatively simple models with a sound statistical underpinning. The associated uncertainty estimation and figures of merit are thoroughly covered in several official documents. However, univariate model predictions for unknown samples are reliable only if the signal is sufficiently selective for the analyte of interest. By contrast, multivariate calibration methods may produce valid predictions also from highly unselective data. A case in point

is quantification from near-infrared spectra. With the ever-increasing sophistication of analytical instruments inevitably comes a suite of multivariate calibration methods, each with its own underlying assumptions and statistical properties. As a result, uncertainty estimation and figures of merit for multivariate calibration methods has become a subject of active research, especially in the field of chemometrics.



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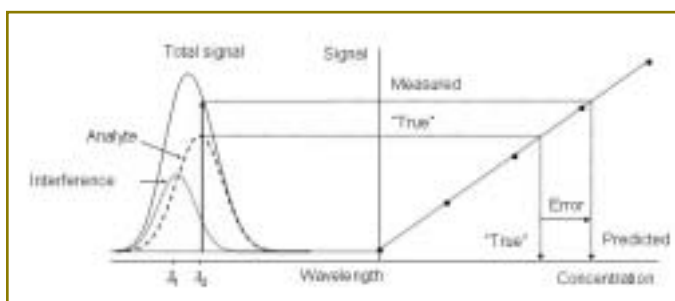


Illustration of how a univariate model will lead to severely biased predictions when unsuspected interferences give a variable contribution to the signal, whereas multiple measurements may permit accurate prediction in such a situation.