

UniQuant[®] 5

a unique concept in XRF analysis

compared with the previous version

■ **FILE STRUCTURE**

User specific data are all in all folders. This enables easy data interchange by email in case of application support or intracompany data exchange. You may use more than one USER folder, for example one for exercise and experimenting with UniQuant features. A USER folder may be win zipped and sent by e-mail to a colleague (UQ user) at another site of your company for comparing methods/results OR may be sent to us for working in parallel in case advice is needed. After placing this folder on the hard disk, one may instantly switch between users in UniQuant, even when another X-ray anode is used.

■ **IMPROVED FUNDAMENTAL PARAMETER (FP) DATA**

Improved fixed tube spectra and mass absorption coefficients based on practical measurements.

■ **PARENT-DAUGHTER PRINCIPLE**

Enabling highest possible accuracy's for each family of samples. New (fast) calibrations are made with a few standards using the PARTENT-DAUGHTER principle. Unlike with conventional methods, a new calibration needs no longer be done from scratch. The new calibration can use data from a calibration for other samples. These data are in a list of instrumental sensitivities, Kappa's. A daughter Kappa list readily derived from a parent list requiring only one or a few standards. The new list differs only slightly from the parent list, thus accounting for specific heterogeneity effects.

■ **REPORTING of ALTERNATIVE LINES**

Next to the primary line, the alternative line is reported by function key F4. For the first time both lines reporting concentration can be seen with both there calculated estimated error.

■ **CALCULATING CONCENTRATIONS OF USER DEFINED COMPOUNDS**

This feature enables to set a compound number (Material Code 1..64) in UniQuant's Intensity List in a new column, marked ##. In the Intensity List, a compound can be specified for any of the analytical lines. User defined compounds are calculated stoichiometrically from one of the analyzed compound elements. Examples of compounds are sulfides and stearates. If a compound gives more than one XRF feasible line, the other line(s) may be use for a "second opinion" or for calculating a surplus as element or oxide. In addition to OXIDES, the user can define more compounds, such as sulfides or stearates, such that use is made of stoichiometry, just as with calculating SiO₂ from SiKa. In this way the concentration of the not bounded sulfur in a sample containing FeS can be calculated.

■ **PROVISION FOR THE INFLUENCE OF SUBSTRATE ON THIN LAYERS**

Previous versions of UniQuant calculated the Mass / area or thickness % Concentrations Based on XRF intensities from layer elements. UniQuant 5 also employs the attenuation of intensity from a substrate element.

■ **TEMPLATES (offline as well as online)**

Use of predefined settings for routine samples based on a dedicated kappa list, data like the chemical state of the sample, weight, height, preset dilution material, assigned compounds, fixed Background settings and more.

■ **USE OF LiBr OR Li ADDITION DURING FUSION**

Those additions are applied in cases where samples are otherwise difficult to fuse with the flux. During fusion, part of the LiBr (or LiI) is lost. That loss is variable, reason why LiBr cannot simply be seen as part of the Diluent (flux). The variable amount of LiBr (or LiI) is to be determined as if it were part of the sample. Line overlaps caused by Br or I are taken into account. At the end of the calculation, UniQuant will subtract the concentration of LiBr (or LiI) from the sum of concentrations and re-normalize the concentrations as if LiBr were not present.

■ **UNIQUANT ON-LINE**

The on-line mode is an automated procedure with an absolute minimum of user intervention. After giving a measure command, the intensities will be automatically exported, imported, calculated and reported. On-line applies only to unknown samples (JOBS), not to calibration standards. The use of catch weights (sample mass and flux mass) is fully supported. This automated procedure may be convenient where the Spectrometer-UniQuant system is used in a production process. The results are printed or saved in a format that is suitable for further processing by the user's own production control software. The use of templates is required.

■ **IMPROVED BACKGROUND CALCULATIONS**

Based on our 15 year experience with UniQuant, we were able to improve the background calculation algorithm in several areas for best performance. This with solving line overlaps once and for all was much more complicated than deriving the matrix corrections from fundamental parameters directly.

■ **REGRESSION ON IMPURITY FACTORS**

Trace analysis can be optimized by means of a regression calculation on these impurity factors. By using a few standards with defined traces, the averaged impurity factor for a given line is calculated. Impurity factors are to be considered as part of the background. In this way, the sensitivity value (Kappa cps/0.1mg) calculated from a refined trace will provide the same sensitivity as the sensitivity calculated from a concentration as high as 99.99%.

This amongst other features enables highly accurate trace analysis.

■ **ADDITIONAL XRF-LINES**

The AsKa, RhLa, AuLb and PtLb line have been added.

■ **NORMALIZATION TO 100%**

Calculating concentrations with an option "C" is with normalization to 100% and is normally used. New is the option "K" which "Calculates" the concentrations without normalization.

■ **NEW MONITOR PROGRAM**

A new monitor program is available since 2004 January.

This program is based on 9 pure metal disks. Major benefits are:

- Fundamental samples with extreme long use.
- Extreme high reproducibility, without sample preparation errors.
- No damage after sample drop.
- Easy cleaning, without risk of pollution.

MM#	Cal.2xx	El
MM1	Cal.222	Ti
MM2	Cal.223	V
MM3	Cal.227	Co
MM4	Cal.230	Zn
MM5	Cal.240	Zr
MM6	Cal.242	Mo
MM7	Cal.250	Sn
MM8	Cal.274	W
MM9	Cal.279	Au