# **XPS MultiQuant** for Windows



## **XPS MultiQuant**

**Technical Notes** 

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## Introduction

These notes are intended to give XPS MultiQuant users additional information on settings of the operating systems and to help solving issues when the origin of the trouble is outside of the of the program.

Applications of utility programs, assisting the work with XPS MultiQuant, are also described. All software tools, mentioned in this manual, are available in the *XPS MultiQuant Utility programs* package (XMQ-Utility.zip).

The author would be indebted if you let him know any other problems. Comments, suggestions on further development and reports on program bugs are also appreciated.

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## List of recent XPS MultiQuant data files

From Windows Vista and above, the operating system maintains the list of the recent files opened by the various programs separately. To apply this feature for XPS MultiQuant, "pin it" to the Start Menu, as follows:

- Open the Start Menu; click **All Programs** then **XPS MultiQuant** folder.
- Right-click **XPS MultiQuant**.
- Click **Pin to Start Menu**.

When you want to use the list, open the Start Menu and click the small right arrow beside the XPS MultiQuant shortcut. Then you can select a file from the opening right hand side menu, as illustrated in the next figure.

🧾 Notepad 🗟 Calculator	۲	Recent
G Microsoft Office PowerPoint 2007	•	TubeSheets.mqd
🐙 Irtanview 🏧 Command Prompt	,	ThickSheetFoil-sum.mqd
🐻 Paint	•	ThickSheet-dec.mqd
😥 XPS MultiQuant	•	📄 ThickSheet-layer.mqd
		📄 Tube-CN-homogen.mqd
		📄 CNTquant.mqd
		📄 MoSi-ZrO-gran.mqd
		📄 PTFE-TAN. mqd
▶ All Programs		
Search programs and files 🖌	þ	Log off 🕨

The list is rolled, as new files are opened. If you want to keep a file on the list for longer time, you can also pin it to the list.

If items were not added to the *Recent Items* automatically, right click the start button and click **Properties**. On the *Start Menu* tab, select the *Store and display recently opened items in the Start menu and the taskbar* checkbox.

## Searching for XPS MultiQuant data files

XPS MultiQuant data are stored in binary files. However, text items in the file (e.g., title, experiment labels, element symbols, notes; but not the numbers) are stored in original form (ASCII) thus the content of the file can be searched by the operating system or other external programs.

Search can be initiated from the graphical user interface, using the searching facility of the operating system, as illustrated below.



Search can also be done from the command window by the *findstr* command.

```
C> findstr /S /M silicon *.mqd
Cermet.mqd
Contact.mqd
Si-ARXPS.mqd
Si-wafer.mqd
SiN-powder.mqd
SiO2-contam.mqd
SiO2-simulation.mqd
C>
```

Apply the /M switch to list only the filenames and not the found text; and the /S switch searching all subdirectories in the current folder.

In Windows Vista and above, searching and indexing of files are controlled by IFilters. "An IFilter is a plug-in that allows Microsoft's search engines to index various file formats so that they become searchable. Without an appropriate IFilter, contents of a file cannot be parsed and indexed by the search engine." (From Wikipedia)

XPS MultiQuant files do not require special IFilter, however, to make them searchable; their extensions must be added to the *Plain text filter* (query.dll).

These settings can be done by the *SearchFilterView* freeware program written by Nir Sofer (http://www.nirsoft.net/utils/search\_filter\_view.html). It does not require installation or additional DLL files.

SearchFilterView				٢
<u>F</u> ile <u>E</u> dit <u>V</u> iew <u>(</u>	<u>)</u> ptions <u>H</u> elp			
	) -71			
Filename 🕧	Description		File Description	*
🚳 query.dll	Null filter		Content Index Utility DLL	
🚳 query.dll	Plain Text filter		Content Index Utility DLL	
🚳 query.dll	Plain Text filter		Content Index Utility DLL	Ŧ
<			4	
Extension /	Type Name	Description	Content Type	*
🗋 .mk				
1 .mqd	MQDfile	XPS MultiQuant Data		
👔 . mqt	MQTfile	XPS MultiQuant Template	9	
🜔 . mtr	MTRfile	XPS MultiQuant Transmis	sion	
🗋 .odh				Ŧ
23 Filters, 1 Selected		NirSoft Freewa	re. http://www.nirsoft.net	

Select the *query.dll* / *Plain Text filter* in the upper pane (usually the first one, with several entries in the lower pane), and then invoke the **File** / **Add Extension To Filter** command. Type the required extensions (.mqd .mqt .mtr) separated by spaces into the popup window, as illustrated below, and press the **OK** button.

Add extensions to selected	d filter			x
Type one or more extensions the list of the selected filter	at you want t	o add into	the extensi	ions
.mqd .mqt .mtr				*
				~
	Ok	:	Canc	el

## Running programs with elevated privileges

Several actions, like installation or update of a program and also some tasks described in this notes require of running them with elevated privileges, i.e., with administrator's right. To run a program with elevated privileges, right-click its icon and select the **Run as different user** command (not the **Run as administrator**) and enter the name and password of the administrator.

To start an elevated command prompt:

- On Start menu, click All Programs then Accessories.
- Right-click **Command Prompt**.
- Click **Run as administrator**.
- Select "Administrator" in the User Account Control dialog box and type the password.

💡 User Account	t Control
🗿 Do yo	u want to allow the following program to make
	es to this computer?
C:4	Program name:Windows Command ProcessorVerified publisher:Microsoft WindowsFile origin:Hard drive on this computer
To continue, t	type an administrator password, and then click Yes.
	Mohai
	Administrator
	Password
Show <u>d</u> etai	ls <u>Y</u> es <u>N</u> o

#### **Component registration error of XPS MultiQuant**

Sometimes at starting XPS MultiQuant, the *Run-time error '339'* message may be appeared, as illustrated below.



This error is occurred when the registration of one or more components (files with .OCX extension), used by XPS MultiQuant, is missing or corrupted. The error may be unintentionally caused by installation, uninstallation or upgrading of other applications, including parts of the operating system. The name of the involved component may vary. XPS MultiQuant uses the following component files: COMDLG32.OCX, GRAPH32.OCX, HHCTRL.OCX, MSCOMCTL.OCX, MSCOMCT2.OCX, MSFLXGRD.OCX, SYSINFO.OCX and TABCTL32.OCX.

To resolve the error, open a command window with elevated privileges (administrator rights) and re-register the involved component(s) by the following commands.

#### On 32-bit system:

```
C> cd C:\Windows\System32
```

```
C> regsvr32 name.OCX
```

#### On 64-bit system:

```
C> cd C:\Windows\SysWoW64
C> regsvr32 name.OCX
```

Where "*name*" is the name of the component. Repeat the *regsvr32* command for each component involved. In 64-bit Windows, there are two *regsvr32* commands with the same name for the 32 and 64-bit applications thus carefully select the proper folder.

When the *regsvr32* command is performed without elevated privileges, the following error message is displayed: *The module* "name.*OCX" was loaded but the call to DllRegisterServer failed with error code 0x8002801c*". The hexadecimal error code may vary, according to the actual component.

All of the components mentioned above can be re-registered by the *CompReg.bat* command file. **CompReg** can be used on both 32 and 64-bit systems. Also run it with elevated privileges.

## Security warnings

Due to the strong security settings of Windows, the system may ask for confirmation before each program start. It can happen for XPS MultiQuant, Kratos Vision Converter or any other utility. The content of the help files may not be shown as well, as illustrated in the next figure.

💕 Kratos Vi	sion Converter Help	
i	Navigation to the webpage was canceled	*
	What you can try:	
	<ul> <li>Retype the address.</li> </ul>	
		-

To avoid this inconvenience, log in as administrator, run the programs and unselect the *Always ask before opening this file* checkbox in the *Open File – Security Warning* dialog box then press *Open*. You must open each help file (XMQ.chm, VisionConvert.chm) directly and perform the same action.

Open File	- Security Warning						
Do you	Do you want to open this file?						
P	Name:nts\Work\W11\VisionConverter\VisionConvert.chm Publisher: <b>Unknown Publisher</b> Type: Compiled HTML Help file From: C:\Users\Mohai\Documents\Work\W11\VisionConv						
	<u>O</u> pen Cancel						
🔳 Al <u>w</u> a	ys ask before opening this file						
۲	While files from the Internet can be useful, this file type can potentially harm your computer. If you do not trust the source, do not open this software. <u>What's the risk?</u>						

Complete disabling the warning for the potentially unsafe files is not recommended. However, the inconvenience can be circumvented by the following steps. After downloading the compressed archive from the homepage of XPS MultiQuant:

- Right-click the ZIP file, then click **Properties**;
- Select the *General* tab;
- Click the **Unblock**, then the **OK** buttons.
- Decompress the archive and install the program as described in the User's Manual.

This method can also be applied for other involved files (.exe, .chm) as well. After unblocking a file, the security warning and the **Unblock** button will not appear on the *General* tab.

诸 XMQ-760up	od.zip Properties
General Secu	ırity Details Previous Versions
- The second sec	XMQ-760upd.zip
Type of file:	Compressed (zipped) Folder (.zip)
Opens with:	😭 Windows Explorer
Location:	C:\Users\Mohai\Desktop
Size:	3.97 MB (4 173 549 bytes)
Size on disk:	3.98 MB (4 173 824 bytes)
Created:	Today, 15 December, 2016, 19:22:00
Modified:	Today, 15 December, 2016, 19:22:00
Accessed:	Today, 15 December, 2016, 19:22:00
Attributes:	Read-only Hidden Advanced
Security:	This file came from another computer and might be blocked to help protect this computer.
	OK Cancel Apply

#### Hints:

When a file is downloaded from the Internet or e-mail attachment, a small alternate data stream, named *Zone.Identifier*, is added by Windows to mark file as possibly unsafe to run. When the user indicates that they no longer want this confirmation dialog (Unblock), this alternate stream is deleted.

## **Customizing number format**

Appearances of the displayed numbers, like decimal symbol, digit grouping and list separator symbols can be set in the *Region and Language* item of the *Control Panel*. Click the **Additional settings...** button and select or set the wanted items on the *Numbers* tab.

👶 Customize	Format		×
Numbers Cur	rrency Time Date		
Example			
Positive:	123 456 789.00	Negative:	-123 456 789.00
<u>D</u> ecima	al symbol:	•	•
<u>N</u> o. of	digits after decimal:	2	-
D <u>i</u> git gr	rouping symbol:		-
Di <u>g</u> it gr	rouping:	123 456 78	9 🗸
N <u>e</u> gativ	ve sign symbol:	-	•
Negativ	ve number format:	-1.1	•
Dis <u>p</u> lay	leading zeros:	0.7	•
<u>L</u> ist sep	arator:	,	
<u>M</u> easur	rement system:	Metric	-
<u>S</u> tanda	rd digits:	012345678	9 -
<u>U</u> se nat	tive digits:	Never	
Click Reset numbers, c	to restore the system defau urrency, time, and date.	It settings for	r <u>R</u> eset
	(	ок	Cancel Apply

Although the standard decimal mark is point or comma in most of the world, Windows allows using *any* character as decimal separator. The usual list separator is comma, except when the decimal mark is comma. In this case the list separator is typically semicolon but also *any* character can be selected. The recommended standard digit grouping symbol is space but it is preferred to omit digit group separators from texts prepared for machine read.

Generally, it is not necessary to alter the local numeric format before reading text files or pasting text into XPS MultiQuant, except at some unusual combination of delimiter characters. Changes of numeric format takes effect after restarting XPS MultiQuant.

## **Opening data source files for import**

A simple way to supply input data, to open the data file with its native reader program, copy the required part of the file and paste it into XPS MultiQuant. The following table summarizes the common file types which can be served as sources of data for XPS MultiQuant; and the capabilities of some widely known programs to open them.

File types	Microsoft Excel	Microsoft Word	WordPad	Notepad	AkelPad	Origin	Adobe Reader	Adobe Acrobat	Web browsers
Column selection	$\checkmark$	$\checkmark$			$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	
Copy as cells	$\checkmark$	$\checkmark$	$\checkmark$			$\checkmark$		$\checkmark$	
Excel workbook	$\checkmark$					$\checkmark$		$\checkmark^1$	
Data Interchange Format	$\checkmark$								
Origin project						$\checkmark$			
Word document table		$\checkmark$						$\checkmark^1$	
text		$\checkmark$						$\checkmark^1$	
Rich Text Format table		$\checkmark$	$\checkmark$					$\checkmark^1$	
text		$\checkmark$	$\checkmark$					$\checkmark^1$	
Text files Windows, DOS	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$		$\checkmark$	$\checkmark$
Unix, Linux	$\checkmark$	$\checkmark$	$\checkmark$		$\checkmark$	$\checkmark$		$\checkmark$	$\checkmark$
Macintosh	$\checkmark$	$\checkmark$	$\checkmark$		$\checkmark$	$\checkmark$		$\checkmark$	$\checkmark$
Portable Document Format							$\checkmark$	V	$\checkmark^2$
HTML document table	$\checkmark$	$\checkmark$						$\checkmark$	$\checkmark$
text	$\checkmark$	$\checkmark$						$\checkmark$	$\checkmark$
Copied as cell-structured text			en Micr	osoft C	Office is	s availa	ble		

Copied as cell-structured text  $^{1}$  Wi Copied as delimited text  $^{2}$  Wi

<sup>2</sup> When plug-in is available

In the cell-structured text delimiters are TAB characters, while in other delimited text, the delimiters can be comma, semicolon, consecutive spaces or any other character selected in Windows. Data copied from XPS MultiQuant is also cell-structured.

WordPad and Notepad are part of the Windows operating system. For the Excel, Word and Origin files, free viewer programs are available, which allow to copy data. For the plain text files, several free text editors can also be selected (AkelPad, NoteTab Light, VIM, etc.).

Column selection, when available, is usually performed by holding down the ALT key while dragging the mouse pointer over the text.

## **XPS MultiQuant file types**

The technical characteristics of the various files and file types used by XPS MultiQuant are described here.



#### XPS MultiQuant Data files (\*.mqd)

Data files are binary. XPS MultiQuant creates, reads and writes them. The text within the file is stored as ASCII characters, not Unicode. When an existing data file is overwritten, the original file is renamed to \*.mqd.bak. If saving was successful, the backup file is deleted; if an error occurred, it is kept and renamed to \*.mqd.save.



#### **XPS MultiQuant Template files** (\*.mqt)

Template files, similar to data files, are binary. XPS MultiQuant creates, reads and writes them.

## **XPS MultiQuant Transmission files** (\*.mtr)

Transmission files are ASCII text. XPS MultiQuant reads and writes them. New files can be created by Notepad or other plain text editors. The structure of the file is described in the *XPS MultiQuant User's Manual*. Decimal separator is point, item separator is comma or semicolon. The line terminator is CRLF (carriage return, line feed). When a transmission file, containing Unicode characters, is opened for calculation, its content will be unchanged but when opened in the internal editor, it is converted and saved as a simple text (ASCII) file.

#### **XPS Reduced Data Exchange files** (\*.mqx) Exchange files are ASCII or Unicode text

Exchange files are ASCII or Unicode text. XPS MultiQuant reads and, in case of successful interpretation, deletes them. The files can be created by Vision Converter or any other capable program. The structure of the file is described in the XPS *Reduced Data Exchange File Developer's Manual*. Decimal separator can be any character as set in Windows (usually point or comma), regardless of the current locale settings. Line terminator characters can be LF, CR or CRLF, thus files written under DOS, Windows, Unix, Linux or Macintosh operating systems can be read without conversion.



#### XPS MultiQuant Library (XMQ.lib)

The library file is binary, located in the application folder. XPS MultiQuant reads it. Generated by the XPS MultiQuant Librarian program.



#### **XPS MultiQuant Workspace** (XMQ.mqw)

The workspace file is ASCII text, located in the application folder. XPS MultiQuant creates, reads and writes it. Users should not modify this file.

#### **Encoding of text files**

The text files are usually simple ASCII files but ones with UTF-32LE (Unicode Transformation Format, Little Endian), UTF-32BE (Big Endian), UTF-16LE, UTF-16BE and UTF-8 encoding can be also read without previous conversion. Files may have Byte Order Mark at the beginning.

## **Display issues**

#### Multiple display systems

On multiple display systems the splash window is always displayed on the primary monitor; although XPS MultiQuant is opened on the same one, where it was closed before.

When the program is displayed on the secondary monitor, the tooltips of some controls may be shown on the primary one, as illustrated below.

	🔋 XPS Multi	Juant		
2012/06/06/06	File Edit V	iew Tools Window Help		
Level 1 error(s)	Model           Name           Link to           Mol. we           Density           0           1           2           3           1           2           3           1           2           3           1           2           3           0           4           0           3           0	Model Summary Model type Elements Layers Islands Number of equations Number of necessary elements within islands • Missing IMFP data	Layers-on-Sphere 4 2 3 3 ·	□       Si         ulk       Omit         Si3N4       40.31         3.440       3.00         4.00       26.80         21.30       3.00

#### Wizard What's This? help

The *What's This?* help text for the *Wizard* window, when invoked by the **Help** menu command and mouse click, will be displayed behind the window (left). Activate help for the wizard by the F1 key to show it in front of the window (right).



## Uninstalling XPS MultiQuant

After removing XPS MultiQuant by its uninstaller program, some updated files may remain in the *XMQ* folder in the *Program Files* or *Program Files* (*x86*) system folder. In this case the *XMQ* folder cannot be deleted either. To remove all stuck files and folders of XPS MultiQuant, apply the *DeleteXMQfiles.bat* command file, as follows.

- If the *Vision Converter* program is installed, run its *Uninstall.bat* command file. If the latter were not done, the shortcut to the program on the start menu remains, although the *Vision Converter* files will be deleted by the *DeleteXMQfiles.bat*.
- Uninstall XPS MultiQuant by the **Control Panel / Programs and Features / XPS MultiQuant** command. Never omit this step, because only the uninstaller program can properly remove the registrations of the component files.
- Run the *DeleteXMQfiles* command file with elevated privileges. The batch pauses at each deleting step thus the user can control the process. Press any key to continue or terminate it by the close button of the command window at any step.

The uninstaller program removes the values and data of the registry entries of XPS MultiQuant but the keys at the highest level (enumerated in the User's Manual) are still remained. To remove all registry entries, use the *DeleteXMQregistry.reg* registration file.

- Right click the *DeleteXMQregistry* file and select the **Merge** command.
- Enter the administrator password, if requested.
- Click the *Yes* button on the following confirmation message:

Registry	Editor
▲	Adding information can unintentionally change or delete values and cause components to stop working correctly. If you do not trust the source of this information in E:\XMQ\Delete\DeleteXMQregistry.reg, do not add it to the registry.
	Are you sure you want to continue?
	Yes No

The registry items to be removed can be inspected by the **Edit** command.

## Running XPS MultiQuant under other operating systems

Although XPS MultiQuant is developed for Windows, it can also be run on other operating systems, using the *Wine* compatibility layer.

Wine ("*Wine Is Not an Emulator*") is a free and open-source compatibility layer capable of running Windows applications on several POSIX-compliant operating systems, such as Linux, macOS and BSD. Instead of simulating internal Windows logic like a virtual machine or emulator, Wine translates Windows API calls into POSIX calls on-the-fly, eliminating the performance and memory penalties of other methods and allowing you to cleanly integrate Windows applications into your desktop. Ideally, if an application runs fine in Windows, it should run fine on the same hardware using Wine.

XPS MultiQuant was successfully tested under Ubuntu 18.04 Bionic Beaver Linux and Wine version 3.0.

#### **Installing Wine**

The easiest way to use a precompiled binary package for your operating system/distribution. The packages, including detailed instructions, are available in the homepage of Wine (https://www.winehq.org/). Many Linux distributions come with an included Wine package, but due to Wine's rapid development rate these may be old or broken versions.

#### Installing XPS MultiQuant

Most binary Wine packages will associate Wine with .exe files. If that is the case, you should be able to simply double-click on the *Setup.exe* file of XPS MultiQuant in the file manager, just like in Windows. You can also right-click on the file, choose "Run with", and choose "Wine".

### **Kratos Vision Converter utility**

The most time consuming task when using of XPS MultiQuant, is to type element and intensity data of experiments. Transferring larger amount of data by this way is tedious and may be the source of potential errors. Although the XPS Reduced Data Exchange file is suggested to solve this task but this format is not yet widely applied.

Another possible solution may be, to interpret the quantification reports prepared by most of the XPS data processing systems. These reports can usually be saved as simple text files. The files can be converted to XPS Reduced Data Exchange files, which can be read by XPS MultiQuant.

Users of different XPS data processing systems are kindly asked to send as many as possible types of report files to the author of the program, in order to write various converter / import programs for XPS MultiQuant.

📒 К	🚍 Kratos Vision Converter										
File	Options Help										
001											
002		Q	uantific	ation Repo	rt						
003	/export/home/krat	os/data/Y09	/Si-scrx	.dset		Fri Feb	19 13 <b>:</b> 42	:32 2010	_		
004									=		
005											
006	State #0 : Etch T	'ime 0.0	0 second	.8					-		
007											
008	Peak	Position	FWHM	Raw Area	RSF	Atomic	Atomic	Mass			
009		BE (eV)	(eV)	(CPS)		Mass	Conc 🗞	Conc 🗞			
010											
011	0 ls	532.300	1.925	2666.1	0.736	15.999	32.79	32.21			
012	C ls	284.400	1.684	1711.8	0.318	12.011	48.73	35.93			
013	Si 2p	102.800	1.720	757.2	0.371	28.086	18.48	31.86	Ŧ		

A converter program is ready to use for users of the Kratos Vision system.

The *Quantification Reports*, produced by the *Kratos Vision 2* data system can be smoothly converted to XPS Reduced Data Exchange files. These reports are simple ASCII text files. The line terminator characters can be LF (line feed), CR (carriage return) and CRLF characters, thus files written by Vision systems running on Windows or Unix operating systems can be read without further change.

Normally, all lines of the report files are started with six consecutive space characters. Lines beginning with other character combinations are neglected. Thus, comments may be added to the reports and unnecessary lines can be marked easily to omit. Several lines can also be omitted at once by starting the first and last line by two slash (//) characters.

Vision system enters the element symbol and line notation separated by a space character. However, users are allowed to edit the *Name* field (in Vision Processing) without limitations. The program tries to analyze the non-standard name fields as well but the success is not guaranteed. The best practice is to keep the original style and separate the symbol, line and chemical state notations by spaces.

The nominal line energy values and the relative sensitivity factors of the elements may also be included to the Element section by selecting the corresponding items in the *Options* window.



The converted XPS Reduced Data Exchange file contains all the three experiment sections (Intensity, Energy, FWHM). The name of the Vision data file (\*.dset) is written to the Name label. The *State* line entries are processed as follows: The *Etch Time* and *Counter* entries are written to the *Time* labels; The *Angle (Position)* to the *Tilt*, while the *Multipoint*, *Temperature* and *Sample magazine* entries to the *Temperature* labels.

The file to be converted can be selected by several ways:

- browsing by the File / Open... command;
- drag and drop the file into the program's window;
- pasting the Vision report text into the program's window.

After selecting the file, it is processed and listed immediately. The name of the output file is the same as the input one with .mqx extension. If the *Open by XPS MultiQuant* item is selected in the *Options* window, XPS MultiQuant is started automatically and the output file is passed to it. When an XPS Reduced Data Exchange file is successfully interpreted by XPS MultiQuant, it will be deleted. To prevent it, select the *Keep XPS Reduced Data Exchange* file item, which sets the Read-only attribute of the output file.

If the file converted by pasting and it is not opened automatically by XPS MultiQuant, a name for the XPS Reduced Data Exchange file is requested. The Vision report file, which is normally deleted, can also be saved by selecting the *Save Kratos Vision report file* item in the *Options* window.

If the *List XPS Reduced Data Exchange file* option is selected, the exchange file is listed, instead of the input report.

In case of error, the XPS Reduced Data Exchange file is not prepared and an error message is shown, indicating the number of line of the report causing the problem.

## **XPS MultiQuant File Check utility**

The *XPS MultiQuant File Check* utility (XMQverChk.exe) examines and displays the type and the version number of the files related to XPS MultiQuant. Files are identified by their content, not by extension thus files with improper extensions are also recognised. However, the validity of the file is not tested.

🖹 XPS MultiQuant File Check 📃 🗾								
File C:\Program Files\XMQ\Samples\SiN-powder.mq	d							
Type XPS MultiQuant Data file								
Program version 7.21 Open								
Data file version 2.31 Example file 🔽	Browse							

The following file types can be examined:

- XPS MultiQuant Data files (\*.mqd)
- XPS MultiQuant Template files (\*.mqt)
- XPS MultiQuant Transmission files (\*.mtr)
- XPS MultiQuant Library file (XMQ.lib)
- XPS MultiQuant Workspace file (XMQ.mqw)
- XPS Reduced Data Exchange files (\*.mqx)

The version number of XPS MultiQuant program, writing the data or template files, is also shown. The example features of these files are also indicated. Files can be selected either by the *Browse* button or by drag & drop. If a file type is associated with an application (usually *XPS MultiQuant* for data, template and exchange files and *Notepad* for transmission files), it can be opened by the *Open* button.

## **Geometry calculations**

Calculation of excitation – analyser or sample normal – analyser angles of XPS instruments and the calculations of the geometry correction factors on inside or outside of a tube or a dome can be conveniently performed by the *XPS-Angles.xls* Excel 2007 worksheet.

Details are described in chapters "Transforming Angles", "Layers Inside a Tube" and "Layers on Domes" of the user's manual of XPS MultiQuant,

	A	В	С	D	F	G			
1	<b>XPS instrument a</b>	ngle c	alculat	io	n				
2		-							
3	Spectrometer geometry								
4	Elevation angle of excitation	α	25.0	°					
5	Azimuthal angle of excitation	β	180.0	•					
6	Elevation angle of analyser	Y	90.0	•					
7	Azimuthal angle of analyser	δ	0.0	•					
8	Tilt angle set on Y axis	ω	0.0	•					
9									
10	Excitation source to analys	ser angle							
11	A = 1 / sin α. 2.3662								
12	B = 1 / sin γ								
13	C = 1 / tan α.		2.1445						
14	D = 1 / tan γ		0.0000						
15	$E^2=C^2+D^2-2\;CD\;\mathrm{cos}\;\delta{-}\beta$		4.5989						
16	$\cos \phi = (A^2 + B^2 - E^2) / 2AB$		0.4226						
17	Excitation - analyser angle	φ	65.0	•					
18									
19	Emission angle								
20	A = 1 / sin γ		1.0000						
21	B = 1 / cos ω		1.0000						
22	C = 1 / tan γ		0.0000						
23	D=tan ω		0.0000						
24	$E^2=C^2+D^2-2\;CD\;\mathrm{cos}\;\delta$		0.0000						
25	$\cos\theta = (A^2 + B^2 - E^2) / 2AB$		1.0000						
26	Sample normal - analyser angle	θ	0.0	•					

Enter the measured instrument angles into the green cells; then get the excitation – analyser and emission angles in the red coloured cells.

	A	В	C D	E	F	G
1	Geometry corr	rectio	on for tul	be secti	on	
2		•				
3	Central angle calculat	tion				
4	Tube section height	h	0.134			
5	Tube section width	d	1.000			
6	Tube section central angle	ρ	1.047 rad			
7	Tube section central angle	ρ	60.0 °			
8						
9	Geometry correction	factor o	calculation			
10	Tube section central angle	ρ	60.0 °	~tube	-:(	-i=(-, - <b>P</b> )
11	Angle increment	β	5.0 °	$G_{\alpha} = :$	$\sin(\alpha + p) - s$	<i>sm</i> (α-p)
12	Facet tilt angles	α	α-β	α+β	Gα	<b>G</b> <sub>α</sub> %
13		0	0.0	5.0	0.0872	17.4
14		10	5.0	15.0	0.1717	34.3
15		20	15.0	25.0	0.1638	32.8

	A	В	C D	E	F	G
1	Geometry corre	ectio	on for do	me sec	tion	
2						
3	Central angle calculati	on				
4	Dome section height	h	0.289			
5	Dome section width	d	1.000			
6	Dome section central angle	ρ	2.095 rad			
7	Dome section central angle	ρ	120.0 °			
8						
9	Geometry correction fa	actor o	alculation			
10	Dome section central angle	ρ	120.0 °	⊂ dome	$\frac{2}{2}$	$ain^2(a, B)$
11	Angle increment	β	5.0 °	$G_{\alpha} = s$	$m (\alpha + p) -$	<i>sm</i> (a-p)
12	Facet tilt angles	α	α-β	α+β	Gα	<b>G</b> <sub>α</sub> %
13		0	0.0	5.0	0.0076	1.0
14		10	5.0	15.0	0.0594	7.9
15		20	15.0	25.0	0.1116	14.9

Enter the height and width of the tube or dome sections into the green cells of the upper table to calculate central angle; then enter the central angle into the green cell of the lower table to calculate geometry correction factors for the tube or dome sections.

## **Revoking IMFP correction**

The composition results are already corrected for cross section, angular distribution, analyser transmission, IMFP and perhaps for surface contamination. All corrections should be applied only once thus for subsequent calculations they must be switched off. In some cases IMFP must be applied directly during the new calculation, therefore the previous correction for IMFP must be revoked from the composition results: according to Equations (5) and (6) in the User's Manual, data should be multiplied by the involved homogeneous IMFP. Intensity data in the program are rounded to integer thus to avoid loss of precision, it is advisable to multiply all values by 100 or 1000.

	A B	С	D	E	F	G	Н	J
	Revoking	IM	FP cor	rection	n from	compo	sition	results
1								
2								-
3			Α	В	С	D	E	
4	Composition	1						Enter or paste
5		2						composition data.
6		3						
7		4						
8		5						
9		6						
10								
11	IMFP	1						Paste IMFP data from the
12		2						Applied IMFP window.
13		3						
14		4						
15		5						
16		6						
17								
18	Composition	1						Copy data to the
19	× IMFP	2						Intensity window.
20	× 1000	3						
21		4						
22		5						
23		6						

The homogeneous IMFP data to be revoked can be copied from the *Applied IMFP* window, invoked by the **Show...** command in the *IMFP* tab of the *Parameters* window. These calculations can be easily performed by the **Revoke-IMFP.xls** Excel 2007 worksheet.