



# *Profex User Manual*

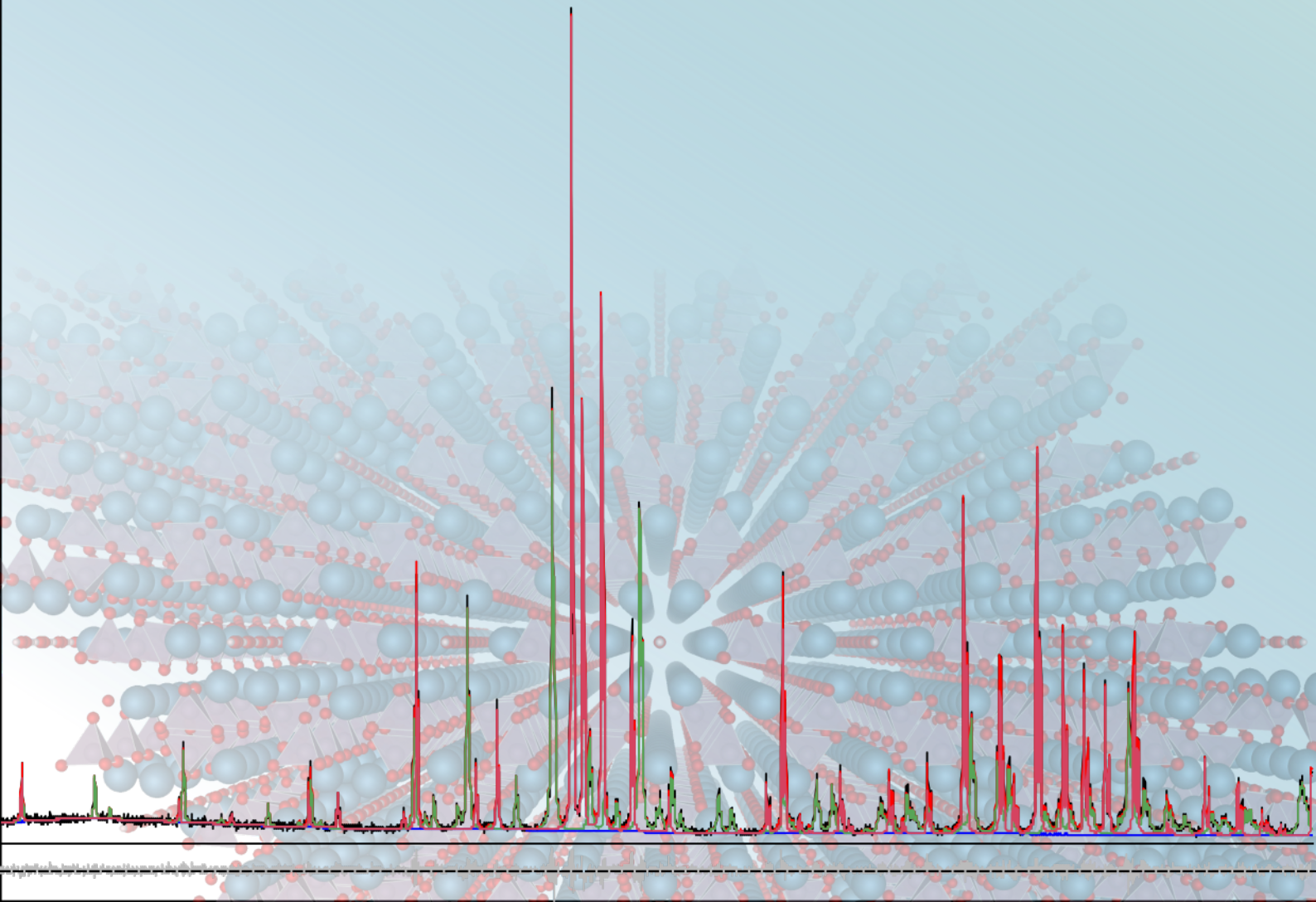
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*Version 4.3*

*Part 1: Installation*

*Nicola Döbelin*

*January 25, 2021*



# *Profex User Manual*

## *Part 1: Installation*

### *Version 4.3*

January 25, 2021

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<https://www.profex-xrd.org>



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## Introduction

Profex is a graphical user interface for Rietveld refinement of powder X-ray diffraction data with the program BGMN [1]. It provides a large number of convenient features and facilitates the use of the BGMN Rietveld backend in many ways. Some of the program's key features include:

- Support for a variety of raw data formats, including all major instrument manufacturers (Bruker / Siemens, PANalytical / Philips, Rigaku, Seifert / GE, and generic text formats)
- Export of diffraction patterns to various text formats (ASCII, Gnuplot scripts, Fityk scripts), pixel graphics (PNG), and vector graphics (SVG)
- Batch conversion of raw data scans
- Automatic control file creation and output file name management
- Conversion of CIF and ICDD PDF-4+ XML structure files to BGMN structure files
- Internal database for crystal structure files, instrument configuration files, and predefined refinement presets.
- Computation of chemical composition from refined crystal structures
- Batch refinement
- Export of refinement results to spread sheet files (CSV format)
- Context help for BGMN variables
- Syntax highlighting
- Enhanced text editors for structure and control file management and editing
- Generic support for FullProf.2k [2] as an alternative Rietveld backend to BGMN.
- And many more...

Profex runs on Windows, Linux, and Mac OS X operating systems and is available as free software licensed under the GNU General Public License (GPL) version 2 or any later version. The latest version of the program can be downloaded from [3]. This website provides the Profex source code, bundles of Profex and BGMN for easy installation on Windows and Mac OS X (requiring zero configuration), and a default set of crystal structure and instrument configuration files.

# 1 Installation

## 1.1 Windows

Profex is offered for download in four different packages. Installers for 32bit and 64bit systems, and portable bundles for 32bit and 64bit systems. On modern computers (Windows Vista/7/10), the 64bit versions are recommended. The installer uses a regular setup routine allowing to select the install location, as well as which of the Profex and BGMN modules are installed. The portable bundle, on the other hand, contains all modules but does not need installation. Instead, the content can be extracted to any location and Profex can be run from there.

### 1.1.1 Installer setup

The installer setup (Fig. 1) allows to chose the target folder for the installation. Usually the default location is the system's „Program Files“ folder. On the next page, the modules to install can be selected. Note that Profex requires BGMN to work. Unless BGMN is already installed, it is recommended to install at least the BGMN executable files. If selected, BGMN and its related files will be installed inside the Profex program files and will not alter any system environment variables. It can coexist and does not interfere with previous BGMN installations. On the next page, the GPL license must be accepted, which applies to both Profex and BGMN. After selecting the location for the start menu links, click „Install“ to start the installation.

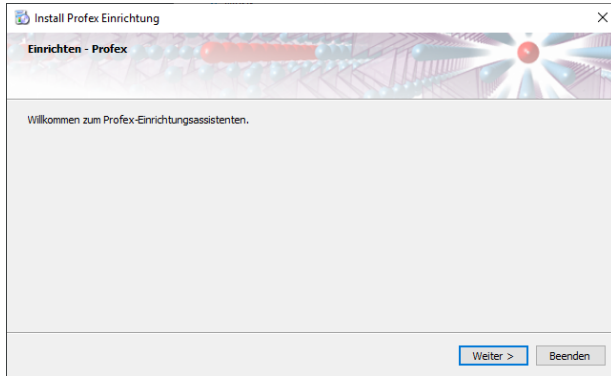
To uninstall, go to the Windows 10 preferences, select „Apps“ and search for Profex in the list of installed applications. Select „Remove“ and follow the instructions to completely remove Profex from the system.

Warning: When uninstalling Profex from the system, the entire program folder will be removed. All device or structure files stored in these folders, including custom ones added manually, will be deleted! Structure and device repositories outside of the Profex installation folder will not be affected by uninstallation.

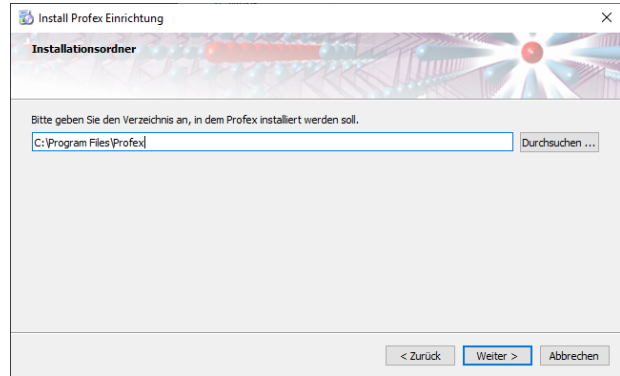
### 1.1.2 Portable bundle

The downloaded archive can be extracted to any location on the computer. Automatic configuration of Profex will be able to locate the BGMN installation if the relative paths of the BGMNwin and Profex-4.3 folders are maintained. Therefore, it is recommended to copy the entire bundle to the same location on the hard disk, as shown in Fig. 2. Follow these instructions to install BGMN and Profex from the portable bundle:

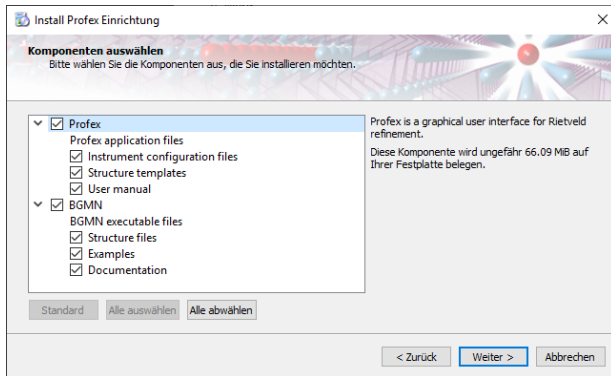
1. Download Profex-4.3.x.zip from [3]
2. Extract the bundle to your harddisk (e. g. C:\Program Files)
3. Run Profex by executing the file profex.exe (e. g. C:\Program Files\Profex\profex.exe)



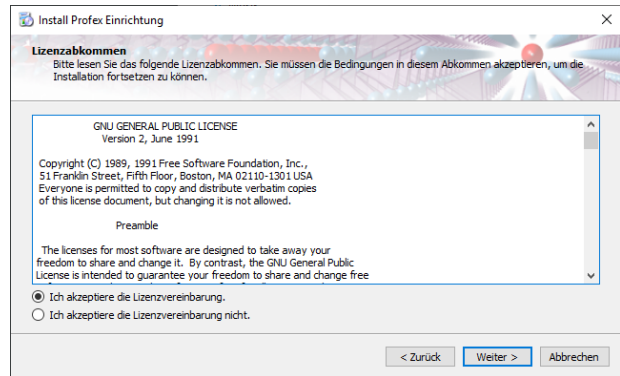
(a) Welcome page



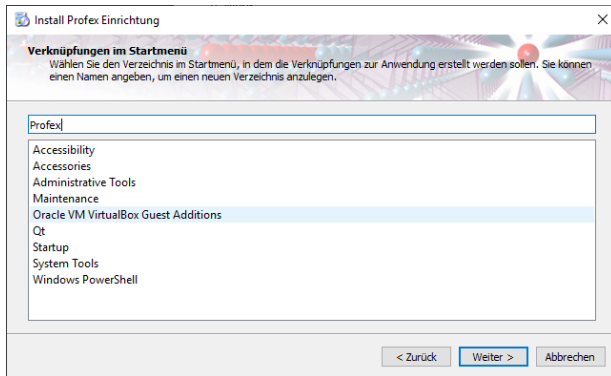
(b) Installation folder



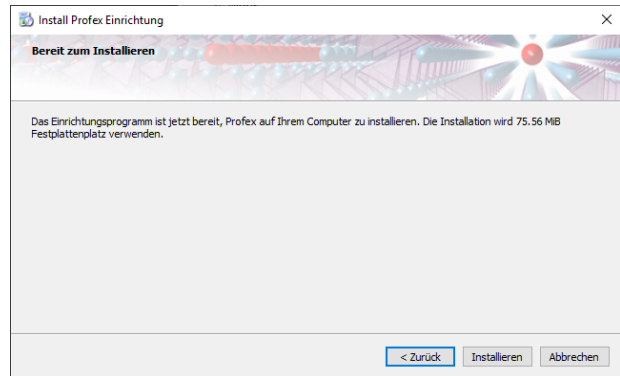
(c) Modules to be installed



(d) GPL license



(e) Start menu entries



(f) Ready to install

Figure 1: The installer setup guides through the installation step by step.

If a previous version is installed on the same computer, running a new portable version will not interfere with the existing installation. Old and new versions can be used at the same time. However, they will share the configuration options, including the locations of BGMN, structure and device repositories. The new version will therefore continue using the repositories of the previous version.

## 1.2 Linux

A binary archive of BGMN for Linux (32 and 64 bit) is available for download on the Profex website [3]. An RPM bundle containing BGMN and Profex is also provided for OpenSuse Leap (64bit). The RPM package installs Profex, BGMN, and a default set of structure and device templates to the `/opt` directory.

Users of linux distributions other than OpenSuse can download and extract the BGMN binary archive and template files, but must compile Profex from the source code.

### 1.2.1 Getting the source

Download the source code archive `profex-4.3.x.tar.gz` from the Profex website [3], extract it to your harddisk and navigate into the source code directory:

```
tar xzvf profex-4.1.0.tar.gz
cd profex-4.1.0
```

### 1.2.2 Compiling from source code

Compiling Profex requires a C++ compiler environment and the Qt toolkit version 5 to be installed [4], including header files. Qt version 5.9 or later is required. The following Qt 5 modules and header files must be installed:

```
widgets, xml, printsupport, sql, svg, qml
```

The package names for these modules depend on the distribution. Some examples for installation commands are given below. On most distributions these commands must be entered with root privileges.

**Ubuntu 16.04:** `apt-get install qtbase5-dev libqt5svg5-dev qtdeclarative5-dev`

**PCLinuxOS:** `apt-get install lib64qt5base5-devel lib64qt5svg-devel lib64qt5qml-devel lib64qt5imageformats-devel`

**OpenSuse Leap 42.1:** `zypper install libqt5-qtbase-devel libqt5-qtsvg-devel libqt5-qtdeclarative-devel libqt5-qtimageformats-devel`

Profex also requires the 3<sup>rd</sup> party libraries zlib [5], QuaZip [6], QCustomPlot [7], and ALGLIB [8]. All libraries are included in the Profex source code archive and linked statically into the binary in order to avoid version conflicts with system-wide installed libraries linked against Qt version 4.

To compile the program run the following commands from the source code directory:

```
qmake -r
make -j 4
src/profex
```

Make sure `qmake` of Qt version 5 is used. If unsure, run `qmake` with the full path. If error messages occur and the program does not start after typing `src/profex`, read the error messages carefully and try to solve all dependency and version problems with your distribution's software repository. `qmake` locations for Qt5 vary among distributions. Some examples are listed below:

PCLinuxOS 64 bit	<code>/usr/lib64/qt5/bin/qmake</code>
PCLinuxOS 32 bit	<code>/usr/lib/qt5/bin/qmake</code>
OpenSuse Leap 42.1 64 bit	<code>/usr/lib64/qt5/bin/qmake-qt5</code>
Debian 8.0 / Ubuntu 16.04 64 bit	<code>/usr/lib/x86_64-linux-gnu/qt5/bin/qmake</code>
Debian 8.0 32 bit	<code>/usr/lib/i386-linux-gnu/qt5/bin/qmake</code>

### 1.3 Mac OS X

A disk image containing Profex and BGMN for Mac OS X 10.9 or newer is provided for download on the Profex website [3]. The binary requires a 64bit CPU. Visit [9] to find out whether a specific Apple computer uses a 64bit or a 32bit CPU.

Mount the disk image and drag the folder Profex-BGMN to the Applications folder. The file and directory structure of the bundle is explained in section 4. Then run the application „Profex-BGMN/profex“. The automatic setup routine (section 2) will find the BGMN installation and the structure and device directories.



```

Profex-4.3.x.zip
├─ Profex-4.3.x
│  ├─ profex.exe
│  ├─ ...
│  └─ BGMNwin
│     ├─ BGMN.EXE
│     └─ ...
├─ Structures
│  └─ *.str
├─ Devices
│  └─ *.geq / *.ger
│  └─ *.sav / *.tpl
└─ Presets
   └─ *.pfp

```

(a) Structure of the bundle archive.

```

C:\Program Files\Profex
├─ Profex-4.3.x
│  ├─ profex.exe
│  ├─ ...
│  └─ BGMNwin
│     ├─ BGMN.EXE
│     └─ ...
├─ Structures
│  └─ *.str
├─ Devices
│  └─ *.geq / *.ger
│  └─ *.sav / *.tpl
└─ Presets
   └─ *.pfp

```

(b) Structure on the hard disk.

Figure 2: When extracting the Profex portable bundle for Windows to the hard disk, automatic setup will only be successful if the BGMNwin and Profex-4.3.x directories are copied to the same location, for example to a directory named C:\Program Files\Profex.

## 2 Setup

### 2.1 Automatic setup

When starting Profex for the first time, the program will try to locate the BGMN installation directory and structure, device, and preset repositories automatically. Automatic configuration will also be executed later if the configured paths are invalid. It is therefore possible to force automatic setup later by deleting the paths to BGMN and the database directories in the preferences dialog, followed by closing and starting Profex. Automatic setup is platform specific. The locations scanned automatically are listed below.

The BGMN backend and repository configuration can be customized in the preferences dialog (Fig. 3). The default setting for the BGMN backend location is inside of the Profex application bundle. For most users this is the preferred setting, because Profex will automatically detect the new BGMN installation when the path changes, for example after updating Profex. Advanced users may prefer to use a different BGMN installation. In that case, check the option „Use custom BGMN installation” and provide the correct paths to the executables.

Automatic repository configuration sets up two different repositories for structure files, device files, and preset files (Fig. 3). One of each is located inside the application bundle and contains the files included in the Profex bundles. The other location is outside of the bundle, the specific location depends on the operating system. Users should store their custom files in the repositories outside of the bundle, so they do not get accidentally deleted when Profex is upgraded to a new version.

Important: After changing the location or content of the structure file repositories in the preferences dialog, call „Tools → Index structure files” to update the internal structure database.

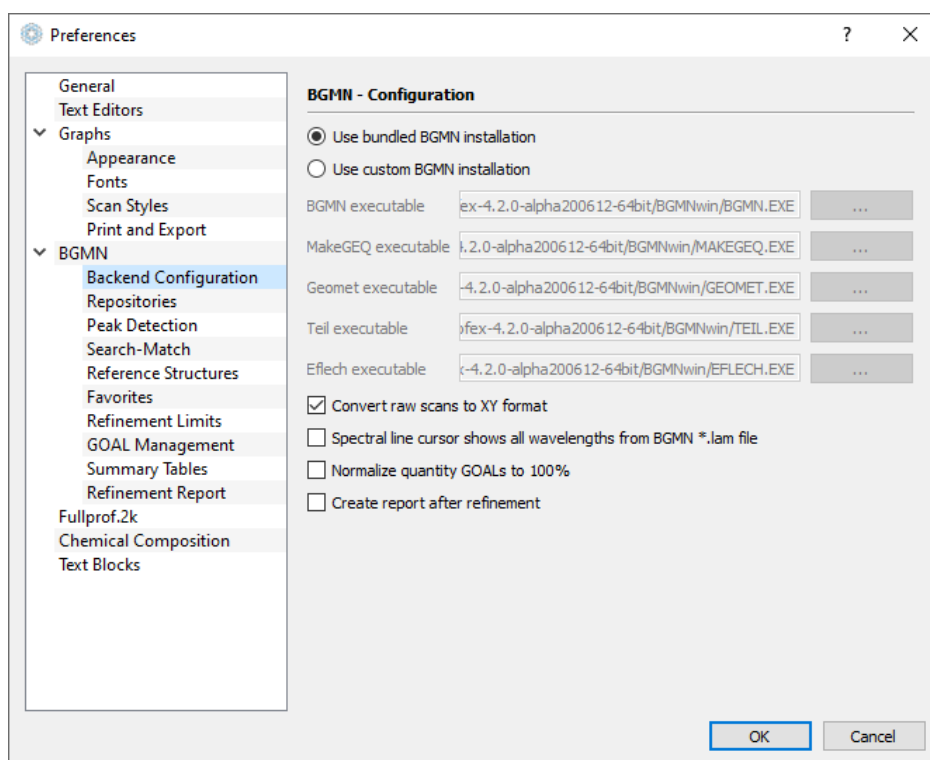
#### 2.1.1 Windows

Three directories named „Structures”, „Devices”, and „Presets” are expected to be located in the directory of „profex.exe”. „BGMN.EXE” is expected to be found in a directory called `BGMNwin` stored next to „profex.exe”. In other words, automatic setup on Windows will work if BGMN and Profex directories are organized as shown in Figure 2.

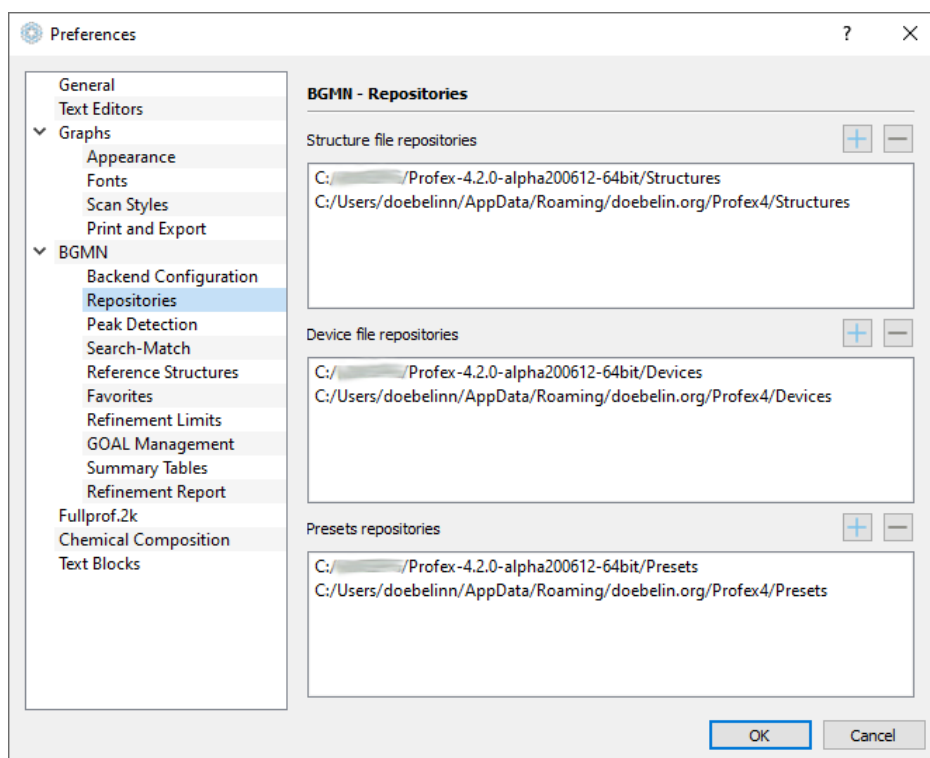
The user repositories outside of the Profex bundle are typically located in:

```
C:/Users/<user>/AppData/Roaming/doebelin.org/Profex4/
```

This is the recommended location for application-specific data on the Windows 10 platform, and it is set up by the Profex repository autoconfiguration. It can be quickly reached from the „Locations” menu in the Profex main window. If a different location for user files is preferred (e. g. on a network-shared drive), it can be configured in the preferences dialog. There is no need to keep the default location for Profex to function correctly.



(a) Backend configuration



(b) Repository configuration

Figure 3: BGMN configuration pages in the preferences dialog.

## 2.1.2 Linux

On Linux, a list of directories is scanned for the executable file „bgmn“. Scanning will stop at the first match. The directories are scanned in the following order:

1. /opt/Profex-BGMN/BGMNwin
2. /home/<user>/BGMN/
3. /home/<user>/BGMNwin/
4. /opt/bgmnwin/
5. /opt/bgmn/
6. /opt/bgmn-4.2.22/
7. /opt/bgmn-4.2.23/
8. /opt/BGMNwin/
9. /usr/bin/
10. /usr/local/bin/

Directories named „Structures“, „Devices“, and „Presets“ will be searched in the following order at:

1. /opt/Profex-BGMN/BGMN-Templates/
2. /opt/BGMN-Templates/
3. /home/<user>/Documents/BGMN-Templates/

The user repositories outside of the Profex bundle are typically located in:

```
/home/<user>/.local/share/doebelin.org/Profex4/
```

This is the recommended location for application-specific data on the Linux platform, and it is set up by the Profex repository autoconfiguration. It can be quickly reached from the „Locations“ menu in the Profex main window. If a different location for user files is preferred (e.g. on a network-shared drive), it can be configured in the preferences dialog. There is no need to keep the default location for Profex to function correctly.

### 2.1.3 Mac OS X

On Mac OS X the BGMN installation and Structures, Devices, and Preset repositories will be scanned relative to the path of the Profex application bundle. Profex expects to find the following files, starting at the position of the Profex application bundle. Note that as of Profex version 4.0, the BGMNwin installation is stored inside the Profex application bundle:

- <location of profex.app>/Contents/Resources/BGMNwin/bgmn
- <location of profex.app>/../BGMN-Templates/Structures
- <location of profex.app>/../BGMN-Templates/Devices
- <location of profex.app>/../BGMN-Templates/Presets

The user repositories outside of the Profex bundle are typically located in:

```
/Users/<user>/Library/Application Support/doebelin.org/Profex4/
```

This is the recommended location for application-specific data on the OS X platform, and it is set up by the Profex repository autoconfiguration. It can be quickly reached from the „Locations“ menu in the Profex main window. If a different location for user files is preferred (e. g. on a network-shared drive), it can be configured in the preferences dialog. There is no need to keep the default location for Profex to function correctly.

## 2.2 Manual setup

The following sections describe how to configure Profex to find the BGMN backend, as well as the structure, device, and preset database directories manually. There are some scenarios when automatic setup will fail and the backend and database directories are not found, or when the automatic configuration is not desired:

- if only Profex was downloaded instead of a Profex-BGMN bundle
- if the Profex and BGMN folders from the bundle were not copied to the same location on the harddisk
- if other structure and device repositories will be used than the ones provided with the bundle. E. g. centrally stored on a network shared drive, or from a previous installation.
- on Linux no bundles are available

In these cases, manual configuration is necessary. Follow these instructions to set up Profex manually:

1. Run Profex and go to „Edit → Preferences ...“.
2. On the page „General“ set the „Default Project Type“ to „BGMN“ (Fig. 4).

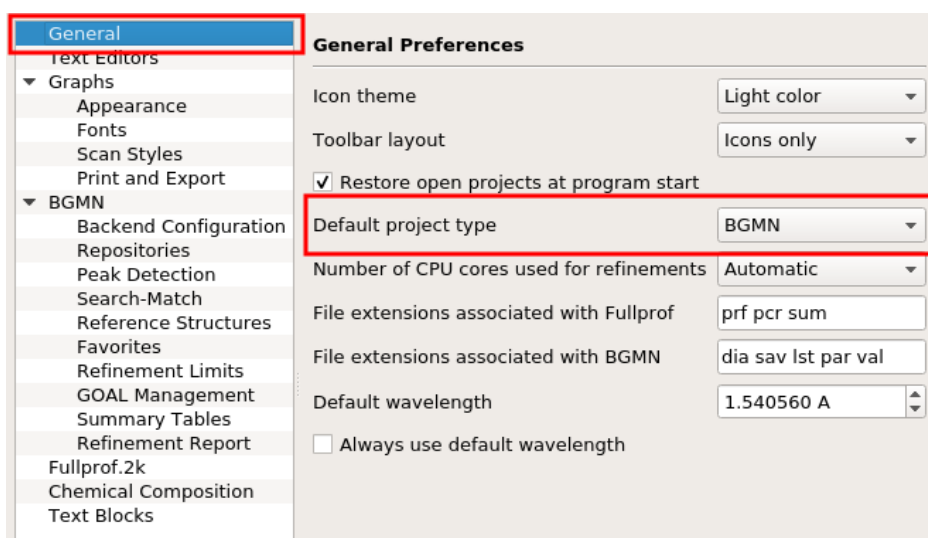


Figure 4: Set the default project type to BGMN.

3. Go to page „ BGMN” and check the configuration of „BGMN Backend”. If auto-detection was successful, the lines for executable files and files directories are not empty (Fig. 3).
4. If the lines are empty, click the button on the right of each line and navigate to the corresponding executable file. The file names depend on the operating system. On Windows, the files are called BGMN . EXE, MAKEGEQ . EXE, GEOMET . EXE, EFLECH . EXE, and TEIL . EXE. On Linux and Mac OS X these files are called bgmn, makegeq, geomet, eflech, and teil.
5. Verify the location of the Structure, Device, and Preset directories. If they are empty or point to the wrong location, click on the button on the right and select the correct directories.

### 3 Structure, Device, and Preset Database

Profex supports databases for crystal structures, device configurations, and refinement presets for the BGMN backend. These databases are directories containing template files. Official Profex-BGMN bundles usually contain default template files for structures and devices. The location of these directories can be chosen freely. For example, installations on several computers can access structures, device files, and presets stored on a network share and maintained centrally. In that case, new structure files, device configurations, or presets will immediately become available to all users using the same database directories. Write access is not required for normal use, only for maintenance. Configuration (automatic or manual) is explained in section 1. Several directories can be specified for each type of repository.

#### 3.1 Structure Template Files

Template files for crystal structures are normal BGMN structure files (\*.str) stored at a central place in the „Structures” database directory. When appending a structure file from the database to a refinement using Profex’ „Add / Remove Phase” dialog  $\pm$ , the file will be copied to the location of the XRD scan. The original file will never be modified.

The following information is relevant when creating new structure files:

- Use the file extension \*.str, other files will be ignored by Profex
- Profex will display the name given after the keyword „PHASE=” in the „Add / Remove Phase” dialog.
- It is recommended to add further information, e. g. an original database code (PDF, AMCSD, COD) after a comment sign (//) trailing the „PHASE=” keyword (see following example). This text will be shown as a comment in the „Add / Remove Phase” dialog.

The following lines show an example of the file „lime.str”.

```
PHASE=CaO // 04-007-9734
Formula=Ca_O
SpacegroupNo=225 HermannMauguin=F4/m-32/m //
PARAM=A=0.4819_0.4771^0.4867 //
RP=4 k1=0 k2=0 B1=ANISO^0.01 GEWICHT=SPHAR2 //
GOAL=GrainSize(1,1,1) //
GOAL:CaO=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=CA+2 Wyckoff=a x=0.0000 y=0.0000 z=0.0000 TDS=0.00350000
E=O-2 Wyckoff=b x=0.5000 y=0.5000 z=0.5000 TDS=0.00440000
```

### 3.2 Device Configuration Files

For each device configuration Profex expects to find four different files in the device database directory. These file names are supposed to have the same file name, but different file extensions:

**\*.sav** Containing the description of the device configuration. To be processed with GEOMET.

**\*.ger** Containing the raytraced profile shape. To be processed with MAKEGEQ.

**\*.geq** Containing the interpolated profile.

**\*.tpl** A sample \*.sav control file for the refinement, not containing any file names or phases (optional).

The \*.tpl file is specific to Profex, all other files will be required by BGMN. More information on the \*.tpl file is given in part 2 of the user manual.

### 3.3 Refinement Preset Files

A refinement preset file allows to quickly create a control file with a certain device configuration file and a set of structures. It is useful for standard refinement always using the same device configuration and structure files, as it allows to set up the control file with a single mouse click. See part 2 of the user manual for more information.



## 4 Bundle File Structure

### 4.1 Windows

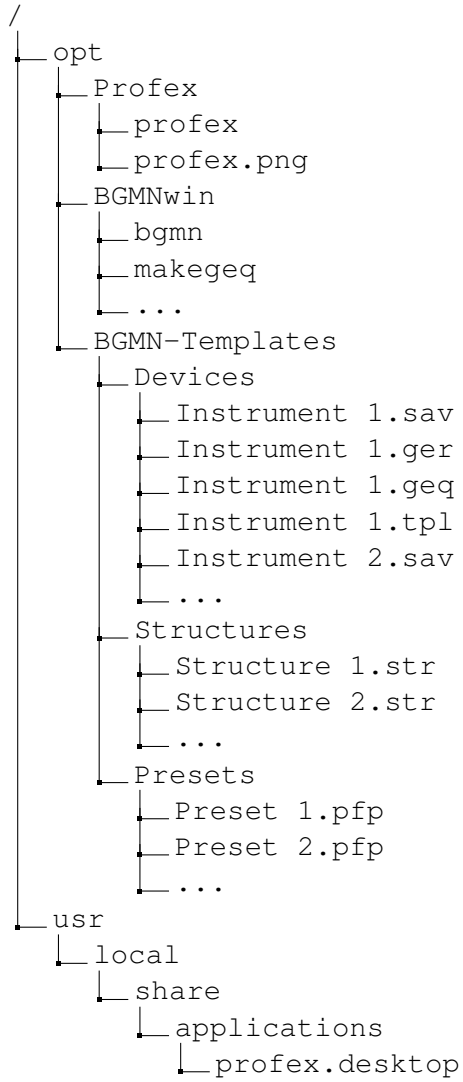
```
Profex-4.3.x.zip
├─ Profex-4.3.x
│   ├── profex.exe
│   ├── ...
│   ├── BGMNwin
│   │   ├── BGMN.EXE
│   │   ├── MakeGEQ.EXE
│   │   ├── ...
│   ├── Devices
│   │   ├── Instrument 1.sav
│   │   ├── Instrument 1.ger
│   │   ├── Instrument 1.geq
│   │   ├── Instrument 1.tpl
│   │   ├── Instrument 2.sav
│   │   ├── ...
│   ├── Structures
│   │   ├── Structure 1.str
│   │   ├── Structure 2.str
│   │   ├── ...
│   └─ Presets
│       ├── Preset 1.pfp
│       ├── Preset 2.pfp
│       └─ ...
```

## 4.2 Mac OS X

```
Profex-4.3.x.dmg
├── Profex.app
│   ├── Contents
│   │   ├── MacOS
│   │   │   └── profex
│   │   ├── Resources
│   │   │   ├── BGMNwin
│   │   │   │   ├── bgmn
│   │   │   │   ├── makegeq
│   │   │   │   └── ...
│   └── BGMN-Templates
│       ├── Devices
│       │   ├── Instrument 1.sav
│       │   ├── Instrument 1.ger
│       │   ├── Instrument 1.geq
│       │   ├── Instrument 1.tpl
│       │   ├── Instrument 2.sav
│       │   └── ...
│       ├── Structures
│       │   ├── Structure 1.str
│       │   ├── Structure 2.str
│       │   └── ...
│       └── Presets
│           ├── Preset 1.pfp
│           ├── Preset 2.pfp
│           └── ...
```

### 4.3 Linux

No bundles are available for Linux. The program needs to be compiled from source, and BGMN templates can be downloaded from the Profex website. A recommended manual installation is shown below.



## References

- [1] <http://www.bgmn.de/>
- [2] <https://www.ill.eu/sites/fullprof/>
- [3] <http://profex.doebelin.org/>
- [4] <http://qt-project.org/>
- [5] <http://www.zlib.net/>
- [6] <http://quazip.sourceforge.net/>
- [7] <https://www.qcustomplot.com>
- [8] <http://www.alglib.net>
- [9] <http://support.apple.com/kb/ht3696/>

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