Monochromator Control Software

User Manual

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MMCS 0.9.7 GPL-3.0

McPHERSON

7A Stuart Road - Chelmsford, Massachusetts 01824
PHONE: (978) 256-4512, 1-800-255-1055
FAX: (978) 250-8625
EMAIL: mcp@mcphersoninc.com
WEB: mcphersoninc.com

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WARNING

Read and understand this user manual before using the Monochromator Control Software. Read and understand the user manuals for each device the Monochromator Control Software can control prior to using or operating the device. Failure to follow the instructions within each manual could result in a dangerous situation.

IMPORTANT NOTICES

ELECTRICAL HAZARD

Electrical equipment can be hazardous if not handled properly. It is important to ensure that all electrical instruments are used with appropriate grounding on power lines, and that electrically powered components are not manipulated or touched unless they have been switched off and disconnected from the power source.

This notice is reiterated in Section 5.4.

DANGER

Mechanical equipment can cause injury if interacted with while in motion. All equipment must be powered down prior to any physical interaction with the equipment.

WARNING

In an emergency, the power should be disconnected from the device. Do not rely on the software in an emergency.

NOTICE

McPherson Inc. will not be held liable for any harm or damages caused by the equipment if the instructions contained in the respective manual(s) are not properly followed, or if the repairs are performed by personnel who are not trained or licensed by the company. It is the user's responsibility to follow all instructions and use the equipment in accordance with the manufacturer's guidelines.

Please see Section 5 for software-related disclaimers and legal information.

1. INTRODUCTION

1.1. OVERVIEW OF MMCS SOFTWARE

The Monochromator Control Software (MMCS, or "the software") is designed as a modern replacement for the original software, McPherson Spectrometer Control Software, written in LabVIEW. MMCS is developed as an open-source project and welcomes contributions adherent to the GNU Public License v3.0 and Section 7. The project is hosted at `github.com/mitbailey/MMC` , where the most recent source code, executable, documentation, and user manual is available. This soft-

ware is offered free of charge without any warranties or fitness for a particular purpose.

1.2. SYSTEM REQUIREMENTS

The software executable requires the use of 64-bit Windows 7, 10, or 11; it is important to note that as of the time of writing the executable has been validated exclusively on Windows 10 and 11.

For advanced users, the code can be compiled and run on any environment capable of running Python 3.9.7, although older versions of Python may work. Due to its use of Qt5, MMCS's additional hardware and software requirements derive from Qt5 (`qt.io`) and PyQt5 (`riverbankcomputing.com/software/pyqt`). For more information about running the program without the executable or interacting with the source code, please see Section 7.

1.3. SUPPORTED HARDWARE

The software supports most instruments from McPherson, with the exception of some older models since they do not include a home switch and are therefore incompatible.

The following motion controllers and detectors are supported:

Motion Controllers

- **KST101** & **ZFS25B** (USB) ThorLabs K-Cube and Motor
- **McPherson 786A-4** (RS-232) Motor Controller (`mcphersoninc.com/pdf/789A-4.pdf`)
- **McPherson 792** (RS-232) Motor Controller (`mcphersoninc.com/pdf/792.pdf`)

Detectors

- **SR810** (RS-232) Stanford Research Systems Lock-In Amplifier
- **SR860** (RS-232) Stanford Research Systems Lock-In Amplifier
- **KI6485** (RS-232) Keithley Instruments Picoammeter

1.4. GETTING STARTED

1.4.1. REQUIREMENTS

- 64-bit Windows 7, 10, or 11.

1.4.2. DEPENDENCIES

- ThorLabs' Kinesis drivers package

  - Kinesis 64-bit Software for 64-bit Windows: https://www.thorlabs.com/software_pages/ViewSoftwarePage.cfm?Code=Motion_Control&viewtab=0
  - Installed in `C:/Program Files/Thorlabs/Kinesis` (as is default).
  - The Kinesis software MUST be run at least once prior to starting MMCS.

Advanced users running directly via source code will also need Python 3.9.7.

1.4.3. DOWNLOADING

The latest version of the software is available on the releases page at github.com/mitbailey/MMC/releases . Expanding the *Assets* dropdown will reveal the executable and zipped source code downloads. Extract the archive to a convenient location.

1.4.4. USAGE

The executable is available within the MMCS zip archive included with each release. Download and extract the archive to access and run MMCS.exe.

The program can be run at any time by double-clicking on *MMCS.exe* and does not require installation.

Before first run (one-time only):

- Unblock `Python.runtime.dll`:
  - 1). Enter the software's folder.
  - 2). Locate the file `Python.runtime.dll`.
  - 3). Right click the file; click "Properties".
  - 4). Check the "Unblock" checkbox near the bottom.
  - 5). Click "Apply"; click "OK".

1.4.5. ON STARTUP

The program will, on startup, perform a number of tasks:

- Create `config.ini` within the program's directory if one does not already exist, or if it is improperly formatted.
- Present the user with the Device Manager window.

Once the communications ports and connected devices have been selected, the *Accept* button has been pressed, and the program has successfully established communication with the devices, the Main Window will be shown and the Device Manager will be automatically closed. See Section 2 for additional details.

1.5. ADVANCED USAGE

1.5.1. SOURCE CODE

The source code can be downloaded either by downloading the *Source code (zip)* file and extracting its contents or by cloning the **`github.com/mitbailey/MMC`** repository.

Python is required to run the program from source code. This can be done by opening a Python interface in the program directory and executing `python mmc.py`.

1.5.2. COMPILATION

The source code can also be optionally compiled and then run. This can be done in one of two methods: one-file and one-directory. The one-file method will produce one executable which is smaller, but slower at startup. The one-directory method creates a directory of files which is larger, but significantly faster to start. See the `requirements.txt` file, included with the source code, for the required Python modules. Detailed compilation steps are listed below.

Compilation Instructions - One File

```
pipenv run pyinstaller mmc.spec
```

Outputs MMC/dist/mmc.exe

Compilation Instructions - One Directory

Prerequisites:

PyQtWebEngine, pipenv

```
pip install PyQtWebEngine
pip install pipenv
```

Pipenv Setup:

```
cd MMC
pipenv install requests
```

Compilation:

```
pipenv run pyinstaller mmc.spec
```

Outputs MMC/dist/MMCS/MMCS.exe

2. USER INTERFACE

2.1. DEVICE MANAGER

The Device Manager is the first window that will be presented after starting MMCS. Here the user chooses which devices they will run. Once the *Accept* button is

pressed, the software will connect to the chosen devices and the Main Window will be launched. The Device Manager will no longer be accessible during the session.

The Device Manager is split into two sections labeled *Detectors* and *Motion Controllers*. At the bottom of the window is the *Accept* button which, when clicked, begins the device connection process. Also at the bottom of the window is a loading bar which indicates the device connection progress; do not be alarmed if it slows or stops - it may take a moment to establish a connection.

and launches the main user interface window, and a loading bar, which can be used to monitor the current device connection progress.

Within each section is an integer input and two sets of drop-down menus. The integer value indicates how many detectors or motion controllers should be connected - one set of drop-downs will appear for each. A maximum of two detectors and 32 motion controllers is allowed. The drop-down menus should then be used to select the communication port for the device (left) and the type of device which is connected to that port (right).

Once the correct device configuration is selected, press the *Accept* button to begin device connection and main interface boot-up. This may take a few moments.

When all of the devices are successfully connected, the Device Manager will close and the Main Interface Window (or Main Window) will open.

2.2. MAIN WINDOW

The Main Window is split into the following four distinct sections: a scrollable *Device Control* area in the top left, a *Data Record* showing all data collected during this session in the bottom left, graphs of collected data on the right, and a status area in the bottom. Additionally, this window has a menu bar (File, Edit, View, About, and Help) along the top. Above the *Device Control* area is the *Quick Actions* bar with multiple icons.

2.2.1. QUICK ACTIONS BAR

The quick actions bar is located in the top right above the device control area. It contains a number of icons with their functions listed below:

 To load a command queue from a file click the folder icon.

 To run the last loaded command queue click the bold arrow.

 To home all axes click the home icon.

 To run a monochromator scan press the arrow icon.

 To stop all axes click the stop sign icon.

 The gear / cog icon is not currently used.

🛠 To open the *Machine Configuration* window click the tools icon. This opens a window which allows configuration of the connected device(s) and is discussed further in section Section 2.2.3.

The stop sign button will immediately halt all device movement. However, in an emergency, the power should be disconnected from the device. Do not rely on the software in an emergency.

2.2.2. DEVICE CONTROL AREA

The device control area, located in the top left section, is likely to be the area most frequently used. Here the user is able to control and configure all connected devices. This scrollable area is broken up into the four main axes: *Main Drive*, *Filter Wheel*, *Sample*, and *Detector*.

NOTICE

MMCS version v0.9.7 does not support the McPherson Model 747 Device Controller, which is necessary for filter wheel control. As a result, software-directed filter wheel control capabilities are not available in this version.

Each axis area has a similar layout. At the the top is the title of the area, flanked on the right by a button.

o the right of the port selection drop-down is a area-collapse button, which will display ⮟ when the area is shown, and ⮜ when the area is hidden. Devices will continue to operate when hidden.

Below the axis area title contains the axis-specific controls which enable movement, scanning, and data collection. Manual movement requires entry of the desired resultant position in units, which are marked, in either nanometers or degrees. Pressing the *Move* button will initiate a move to the entered location. The *Home* button is also available to home an axis at any time.

WARNING

Motion-sensitive user interface elements are disabled while a movement has been initiated. No attempt to initiate further movement should be made while the device is in motion. Press the *All Stop* button at any time to halt all movement on the machine. In the unlikely event of a program failure, crash, hang, or other form of communication failure, the HALT command may be delayed or lost; the power to the motors should be disconnected safely to avoid damage or injury.

Scans are available in the Main Drive, Sample, and Detector axes, and require three input values: *start*, *stop*, and *step*. Once the *Begin* button is pressed, the scan

will begin. During the scan the device is commanded to move to, and sample at, a number of locations determined by *start*, *stop*, and *step*. Location values are generated within the closed interval `[start, stop]` with spacing between values given by *step*. The scan includes both the starting and ending positions. Additional scan types *Rotation*, *Translation*, and *Theta2Theta* are available in the *Sample* axis. *Rotation* scans along the rotation axis, *Translation* scans along the translation axis, and *Theta2Theta* scans along the rotation and detector axes simultaneously where the detector axis is moved to two-times the angle of the rotation axis. Finally, the Repeats spin-box can be set to however many additional and identitcal scans the user would like to do after the first.

2.2.3. MACHINE CONFIGURATION WINDOW

The Machine Configuration Window (or Config Window), which is accessed by pressing the *Machine Configuration* 🛠 button above and to the right of the axis controls, is necessary for configuring the specifics of the connected device(s). When pressed, the Config Window will be opened.

The Config Window has the following four axis-specific tabs: Main Drive, Filter Wheel, Sample Movement, Detector Rotation; and two more general tabs Motion Settings and Detection Settings.

In the Main Drive tab, to properly set the **Steps per Nanometer** value, the **System Model** must be selected, **Grating Density** entered, and the *Calculate Steps per Nanometer* button must be pressed prior to closing the window via the *Accept* button. These values should be provided to you specific to your instrument setup.

In each tab is an **Axis** drop-down. This should be used to select which motion controller device controls which movement axis.

In the Motion Settings tab **Move** and **Home** speeds can be adjusted using a multiplier value from 0 to 1.0. Note that the same multiplier entered into both Move and Home may not necessarily result in the same movement speed.

The Detection Settings tab can be used to set the Scan Start Delay, Detection Delay, and how many samples should be averaged together when performing a detection.

2.2.4. DATA RECORD AND SPECTRAL OPERATIONS

The Data Record area lists each scan that has been taken during the current session, enumerated by its start, stop, and step values. The name given to a scan can be changed at any time by clicking on the name box. Additionally, the *Plot* column allows toggling the viewability of a scan on the graph. Data can be deleted by first selecting its entry and then pressing the *Delete Data* button. Likewise, data can be saved by selecting its entry and then pressing the *Save Data* button.

The Σ◀ button can be pressed to expand the Σ Spectral Operations area. Here, scans and operations can be selected to perform math and obtain results. Results are placed in the *Result* tab of the Data Record.

There are two categories of Spectral Operation: Simple, where the latest sample scan is either multiplied, divided, subtracted, or added on a reference scan; and Reflection/Transmittance (Refl/Tran), where a reference and sample detector are run simultaneously.

In the Simple operation, selected by clicking the *Simple* radio button, the reference scan can be selected by first taking a scan, clicking that scan in the Data Record, then clicking the **Set Reference** button. The button will then show the detector and scan currently set as reference, for example D1S0 for Detector #1′s Scan #0. The **Enact** button must then be pressed to enable this operation. **Reset** can be pressed to stop using this operation and reset the selected reference.

The Reflection/Transmittance operation can be chosen by selecting the *Refl/Tran* radio button. You will then be presented with the following:

Sample Detector ÷ (**Reference Detector** × (**Sample Scan** ÷ **Reference Scan**))

Sample Detector: a drop down where you select which detector will act at the sample detector. In the equation, this slot will be filled by the sample detector's latest scan.

Reference Detector: a drop down where you select which detector will act at the reference detector. In the equation, this slot will be filled by the reference detector's latest scan.

Sample Scan: after running a scan and then selecting that scan in the Data Record, pressing this button will set that scan to be permanently set here in the equation.

Reference Scan: after running a scan and then selecting that scan in the Data Record, pressing this button will set that scan to be permanently set here in the equation.

The **Enact** button must then be pressed to enable this operation. **Reset** can be pressed to stop using this operation and reset the selected reference.

2.2.5. DATA GRAPH

The plot automatically shows all scans completed during the current session. Which scans are shown is controlled by the Data Record, discussed in section Section 2.2.4. The *Clear Plots* button can be used to quickly hide all plots.

2.2.6. STATUS AREA

The Status Area shows, from left to right, the current Main Axis position in nanometers, the system status, and a progress bar detailing the completion progress of the current scan.

2.2.7. MENU BAR

The menu bar, located at the top of the Main Window, contains a number of useful utilities and settings. The buttons, options, and descriptions are listed below.

- File
  - Export Config: *Exports the current configuration and input values as a CSV file.*
  - Import Config: *Allows selection of a CSV file which will populate the configuration and values.*
  - Save Current Config: *Saves the current software and device configuration*
- Edit
  - Machine Configuration: *Alternative method to open the Config Window* (Section 2.2.3).
  - Invert measurements: *Multiplies all future measurements by −1.*
  - Autosave Scans: *Automatically saves all scan data to UNIX-timestamped CSV files.*
  - Change Autosave Directory: *Change where auto-logged data is saved.*
  - Preferences: *Unimplemented.*
- View
  - Pop-out Plot: *Unimplemented.*
  - Pop-out Table: *Unimplemented.*
  - Show Main Drive: *Unimplemented.*
  - Show Filter Wheel: *Unimplemented.*
  - Show Sample Movement: *Unimplemented.*
  - Show Detector Rotation: *Unimplemented.*
  - Show Data Table: *Unimplemented.*
- About
  - Source Code: *Opens a link to the GitHub repository.*
  - Licensing: *Opens a link to the GitHub repository.*
- Help
  - Manual: *Opens a link to the GitHub repository.*

3. FEATURES AND FUNCTIONS

3.1. DATA MANAGEMENT

3.1.1. SAVING AND LOADING DATA

Saving and loading collected scan data is covered in section Section 2.2.4.

3.1.2. IMPORTING AND EXPORTING CONFIGURATIONS

Exporting and importing configurations and values is covered in section Section 2.2.7.

3.2. DATA VISUALIZATION

All data is visualized using the Data Graph discussed in section Section 2.2.5.

4. TROUBLESHOOTING AND SUPPORT

4.1. ERROR MESSAGES

Following are lists of known error messages and their probable causes. Any messages received which are not listed here should be reported via the process detailed in Section 7.1. Crashes should also be reported. In Table ref{tab:table1}, the “Sev.” column notes the severity of the issue. INFO indicates an informative message which does not require significant action. WARN indicates an issue that does not require the program to be restarted. CRIT indicates an issue that can likely only be fixed by restarting the program.

Errors 4-7 report an additional message, represented by the %s. These may provide additional insight into the cause of the issue.

Errors			
#	Title, Message	Sev.	Possible Causes
1	Connection Failure No detector was selected for entry #%d.	INFO	Detector not selected.
2	Connection Failure No motion controller was selected for entry #%d.	INFO	Motion controller not selected.
3	Connection Failure Connection attempt has failed!	WARN	Devices are not connected properly.
4	Move Failure Main drive axis failed to move: %s.	CRIT	Communication or connection failure.

5	Move Failure Sample rotation axis failed to move: %s.	CRIT	Communication port fell asleep. Device disconnected.
6	Move Failure Sample translation axis failed to move: %s.	CRIT	Communication port fell asleep. Device disconnected.
7	Move Failure Detector rotation axis failed to move: %s.	CRIT	Communication port fell asleep. Device disconnected.

4.2. TROUBLESHOOTING COMMON ISSUES

Issue 1

The program crashes on startup.

Solution 1-A

Some systems may require that `Python.Runtime.dll` is ‘unblocked’ manually. To do this:

1). Navigate to `MMCS\pythonnet\runtime`

2). Right-click the file `Python.Runtime.dll` and select *Properties*.

3). Check Unblock in the bottom right-hand corner.

Solution 1-B

Some systems may require administrative privileges to run the program. Right click `MMCS.exe` and press “Run as Administrator.

Solution 1-C

Ensure that the ThorLabs Kinesis Software is installed as discussed in Pre-Requisites.

4.3. CONTACTING SUPPORT

When encountering issues with the software, we recommend visiting github.com/mitbailey/MMC/issues first. However, we strive to provide our customers with the best support possible, and we are always happy to help. If you have any questions

or concerns, please don't hesitate to reach out to us. We are available Monday through Friday, from 9:00 AM to 5:00 PM Eastern Time.

Please see Section 6.2 for details.

4.4. UPDATING THE SOFTWARE

5. LICENSE AND LEGAL INFORMATION

5.1. SOFTWARE LICENSE

Monochromator Control Software is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

Monochromator Control Software is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with Monochromator Control Software. If not, see `https://www.gnu.org/licenses/gpl-3.0.en.html` .

5.2. OPEN SOURCE CREDITS

The Monochromator Control Software uses the following:

PyQt5, Copyright 2022 Riverbank Computing Limited, The Qt Company, under the GNU General Public License v3.0.

Qt5, Copyright 2023, The Qt Company, under the GNU General Public License v3.0.

5.3. WARRANTY AND LIABILITY

For information about warranty and liability, please refer to sections 15, 16, and 17 of the GNU Public License. The entire text of the relevant license is given in `License.txt`, the `COPYING` file, and at `https://www.gnu.org/licenses/gpl-3.0.en.html` . For convenience, the relevant sections are shown below:

15. Disclaimer of Warranty.

    THERE IS NO WARRANTY FOR THE PROGRAM, TO THE EXTENT PERMITTED BY APPLICABLE LAW. EXCEPT WHEN

OTHERWISE STATED IN WRITING THE COPYRIGHT HOLDERS AND/OR OTHER PARTIES PROVIDE THE PROGRAM “AS IS” WITHOUT WARRANTY OF ANY KIND, EITHER EXPRESSED OR IMPLIED, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE. THE ENTIRE RISK AS TO THE QUALITY AND PERFORMANCE OF THE PROGRAM IS WITH YOU. SHOULD THE PROGRAM PROVE DEFECTIVE, YOU ASSUME THE COST OF ALL NECESSARY SERVICING, REPAIR OR CORRECTION.

16. Limitation of Liability.

IN NO EVENT UNLESS REQUIRED BY APPLICABLE LAW OR AGREED TO IN WRITING WILL ANY COPYRIGHT HOLDER, OR ANY OTHER PARTY WHO MODIFIES AND/OR CONVEYS THE PROGRAM AS PERMITTED ABOVE, BE LIABLE TO YOU FOR DAMAGES, INCLUDING ANY GENERAL, SPECIAL, INCIDENTAL OR CONSEQUENTIAL DAMAGES ARISING OUT OF THE USE OR INABILITY TO USE THE PROGRAM (INCLUDING BUT NOT LIMITED TO LOSS OF DATA OR DATA BEING RENDERED INACCURATE OR LOSSES SUSTAINED BY YOU OR THIRD PARTIES OR A FAILURE OF THE PROGRAM TO OPERATE WITH ANY OTHER PROGRAMS), EVEN IF SUCH HOLDER OR OTHER PARTY HAS BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES.

17. Interpretation of Sections 15 and 16.

If the disclaimer of warranty and limitation of liability provided above cannot be given local legal effect according to their terms, reviewing courts shall apply local law that most closely approximates an absolute waiver of all civil liability in connection with the Program, unless a warranty or assumption of liability accompanies a copy of the Program in return for a fee.

5.4. IMPORTANT NOTICE REGARDING ELECTRONICS

Electrical equipment can be hazardous if not handled properly. It is important to ensure that all electrical instruments are used with appropriate grounding on power

lines, and that electrically powered components are not manipulated or touched unless they have been switched off and disconnected from the power source.

McPherson Inc. will not be held liable for any harm or damages caused by the equipment if the instructions contained in the respective manual(s) are not properly followed, or if the repairs are performed by personnel who are not trained or licensed by the company. It is the user's responsibility to follow all instructions and use the equipment in accordance with the manufacturer's guidelines.

6. ABOUT US

6.1. MCPHERSON

This software was designed for McPherson and is intended for use primarily with McPherson hardware. For information on McPherson, please visit `mcphersoninc.com` .

6.2. CONTACT INFORMATION

EMAIL: mcp@mcphersoninc.com **PHONE:** (978) 256-4512, 1-800-255-1055

You can send an email to **mcp@mcphersoninc.com** and we will respond to you as soon as possible. If you prefer to speak with someone over the phone, you can call us at **(978) 256-4512** or **1-800-255-1055**.

7. HOW TO CONTRIBUTE

To see the most current rules on contributing to the project, please visit `github.com/mitbailey/MMC/wiki` . The information found on the wiki supersede any information listed within this manual.

7.1. REPORTING BUGS

Prior to reporting any bugs or issues, it is imperative that it is reproducible. Please attempt to recreate the issue, documenting the steps necessary to cause it. All bugs and issues should then be reported using GitHub's issue tracking system at github.com/mitbailey/MMC/issues. Please also export the software's configuration at the time of the issue and be sure to attach it to your issue post (if the issue is a start-up crash or occurs before entering into the main interface window, it is not necessary to include the current configuration). To open a new issue, click on the "New Issue" button and fill out the form using the following issue template and sample:

Issue Template

Title Which is Descriptive of the Issue
Software Version

"Ran from downloaded executable," "Compiled from source code," *or* "Ran from source code."

List the following only if you compiled or ran from source code: Python Version Instructions on how it was compiled or run.

Operating System

(1) List the steps necessary to reproduce the issue you experienced.

Make sure to include what buttons were pressed, values of relevant spin-boxes and drop-downs. Include images if possible.

(2) What happened? Describe the issue.

Describe the issue itself, and what happened immediately afterwards.

(3) List any error messages that appeared.

Be sure to include the text and title of any errors which appeared.

(4) Additional Notes

Anything you think may help us solve this issue.

7.2. REQUESTING FEATURES

All feature requests should include justification including why this feature would help your specific use case and why it would help the community of program users.

To see the most current rules on contributing to the project, please visit **github.com/mitbailey/MMC/wiki** .

7.3. CONTRIBUTING CODE

To see the most current rules on contributing to the project, please visit **github.com/mitbailey/MMC/wiki** .