

# A New "Open Source" Control Program for Single Crystal Diffractometry

Jürgen Kopf

Institut für Anorg. und Angew. Chemie, Universität Hamburg,  
Martin-Luther-King-Platz 6, D-20146 Hamburg, Deutschland  
e-mail: [kopf@xray.chemie.uni-hamburg.de](mailto:kopf@xray.chemie.uni-hamburg.de)

## Introduction

Over the past decade we have been developing diffractometer control software that uses easy to learn pull-down menus, dialog-, alert- and file-selector-boxes. The program Y290 has been developed to control a still very reliable Hilger & Watts (Y290) four circle diffractometer via a new interface, using a 68008 microcomputer for serving the four stepper motors. The software, including the calls for the graphics system, was completely written in FORTRAN77 for an ATARI Mega ST2 [1].

By isolating all modifications required to drive a different diffractometer, it was possible to re-write the same control program for a SYNTEX P21 diffractometer [2]. This program P21 used the so-called "SIEMENS-box" for driving the four DC motors.

Although an ATARI with 1 MB memory and only 8 MHz processor speed is completely sufficient for driving both instruments, a PC version under the operating system Linux was developed.

The new diffractometer control software is now completely written in C++ using the Qt class library, maintained and distributed by the Norwegian company TROLLTECH [3]. Qt is a multi-platform C++ GUI toolkit that is supported on all major variants of Unix/X11 and Microsoft Windows. It is released in two different versions: the Qt Free Edition, which may be used free of charge for developing Free Software ("Open Source"), and the Qt Professional Edition. Since the new program Y290 uses the Qt Free Edition on Linux/X11, the source code is also free software.



Fig. 1: Photograph of the Hilger & Watts (Y290) with operator Cornelia Bretzke and our old ATARI Mega ST2 as control computer at about 1993.

Tab. 1: Listing of file: main.cpp

```
/* File: main.cpp
 * Copyright (C) 1997-2000 by J. Kopf
 * University of Hamburg
 * Revision date: Aug/15/2000
 * Linux-Version: 1.09
 * e-mail: kopf@xray.chemie.uni-hamburg.de
 *
 * This program 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 2 of the License, or
 * (at your option) any later version.
 *
 * This is the main program for the HILGER & WATTS (Y290)
 * diffractometer program.
 *
 * Content of this file:
 * int main(int argc, char *argv[])
 *
 * =====
 * #include "y290widget.h"
 * #include "datatypes.h"
 * #include "y290.h"
 *
 * int main(int argc, char *argv[])
 * {
 *     Application::setColorSpec(Application::CustomColor);
 *     Application y290app(argc, argv);
 *
 *     Y290Widget y290widget = new Y290Widget();
 *     y290widget->setGeometry(50, 20, 940, 570);
 *
 *     y290app.setMainWidget(y290widget);
 *     y290widget->show();
 *
 *     return y290app.exec();
 * }
```

## Explanation of red numbers

- 1) cell-parameter-widget: This widget shows the actual cell parameters.
- 2) file-name-widget: This widget shows the actual file names.
- 3) position-widget: This widget shows the actual position angles of the diffractometer.
- 4) accessory-widget: This widget controls and shows the accessories of the diffractometer.
- 5) message-widget: This widget functions as a message box.
- 6) draw-widget: This widget shows the actual profiles during centering and data collection.

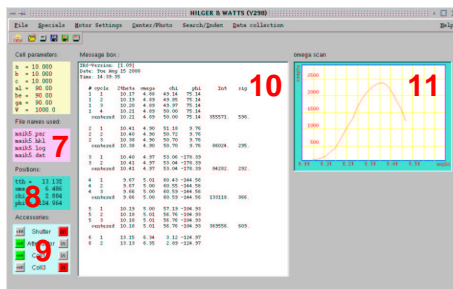


Fig. 3: Screenshot of program Y290 [7] during centering reflection # 6. The centering is done in up to five cycles of omega-, 2theta- and chi-scans. In this Figure you see the omega-profile of this reflection.

## History of our Hilger & Watts (Y290)

Our diffractometer was installed in May 1971. At that time the instrument was equipped with a special DEC interface and a DEC computer PDP8/I with 4K core memory of 12-bit-words. All programs were stored in binary form on a 8-channel paper tape and had to be loaded via a paper tape reader (Teletype ASR33). The loading of the data collection program took over 20 minutes.

In January 1972 a DF32 disk with 32K of 12-bit-words was installed. From that time loading of programs was not necessary anymore, but the changing of programs was very difficult because programs exist only in binary form. There was no operating-system, no assembler and no text-editor. With this configuration it was possible to measure over 1000 crystal data sets.

In February 1982 the DEC PDP8/I was replaced by a PDP8/E with 24K 12-bit-words memory and a 1.6 MB hard disk RK05j and another 3.2 MB hard disk RK05f. The operating-system was OS/8 and TECO was used as text editor. All programs were converted to PALIII assembler, so that changing of programs was now much easier. Also in 1982 a microprocessor Colossus 2.2 with 64 Kbyte memory was connected to the PDP8/E for the data transfer of the diffraction data on 8" floppy disks to the computer center [4].

During the year 1990 the old DEC interface and the original Hilger positioning system with the Moiré-fringe technique and the DC motors were replaced by new 5-phases stepper motors and a new interface [5]. Also a new Oxford Cryostream low temperature device was added to the diffractometer. Since the computer hardware had changed so dramatically, a completely new program for driving the diffractometer was developed in Prospero FORTRAN 77 for an ATARI [6].

Finally in 1997 a Linux Version was started. It was decided to change the programming language again, this time to C++, and to use the Qt class library as Graphical User Interface (GUI) toolkit [7].

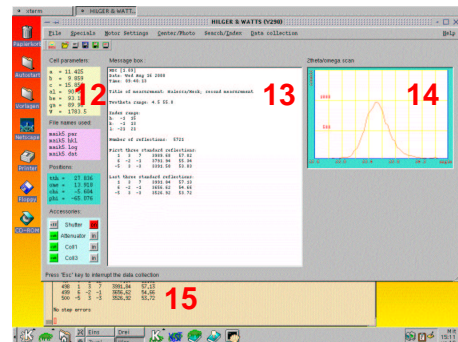


Fig. 4: Screenshot of program Y290 [7] during data collection. In this Figure the whole screen is shown.

## Explanation of red numbers (continued)

- 7) The file-name-widget is now actualized to project: mai k5.
- 8) The position of the omega circle is: 6.486 (compare with draw-widget).
- 9) The shutter is on and the 3mm collimator is set.
- 10) The centering information of the initial reflection search is shown in the message-box. Up to this moment, five reflections are found and centered. There are up to five cycles of omega-, 2theta- and chi-scans. If the precision is exact enough the final intensity of the found reflection is measured.
- 11) The actual omega profile of reflection # 6 is shown during the scan.
- 12) The cell-parameter-widget is actualized to the cell parameters of project: mai k5.
- 13) Actual data collection informations are given in the message box. These informations are: 1.) title of measurement, 2.) 2theta range, 3.) index range, 4.) number of reflections to be measured and 5.) index and intensity informations about the first and the last three standard reflections are also given.
- 14) The online 2theta/omega profile of the last reflection (in this case the third standard reflection) is shown.
- 15) In the terminal window the measured reflections are printed. Every 97 reflections the three standard reflections are measured. After that the stepper motors are checked (no stop errors). In fact, the new Hilger & Watts (Y290) stepper motor system does not have any encoder system.

## Search for volunteers and coworkers

If you are interested in this work and/or you have an old, mechanically reliable diffractometer, please contact me via e-mail or phone me. I'm especially interested in old Syntex/Nicolet (P21 and/or P3) diffractometers with so-called "Siemens-Boxes". In this case there is a good chance to get these diffractometers running again.

## Results

A new "open source" diffractometer control program is now available in C++ using the Qt class library. Qt is a multi-platform C++ GUI toolkit that is supported on all major variants of Unix/X11 and Microsoft Windows. The new version of program Y290 is running over one year very stable without any problems.

## References

- 1) Dirk Abeln, Jürgen Kopf. *The Application of Graphic Desktop Software in Single Crystal Diffractometry*. Abstract PS-02.06.01, IUCr XVI, Beijing, China, 1993.
- 2) Jürgen Kopf, Dirk Abeln. *P21 - A New Graphically Oriented Control Program for Syntex/Nicolet Diffractometers*. Abstract P21-10, ECM 16, Lund, Sweden, 1995.
- 3) Trolltech AS, <http://www.trolltech.com/>
- 4) Jürgen Kopf, Habilitation, University of Hamburg, Germany, 1986.
- 5) Joachim Lange, Hans Buzlaff, *J. Appl. Cryst.* 24, 190-194, 1991.
- 6) Dirk Abeln, Dissertation, University of Hamburg, Germany, 1995.
- 7) Jürgen Kopf, *Y290. Qt-Program for Driving a Hilger & Watts (Y290) Diffractometer*. Linux-Version: 1.09, University of Hamburg, Germany, 2000.

## Acknowledgements

I would like to thank Dr. Dirk Abeln for helping with the ATARI version of program Y290. He also developed the absorption data collection version which is not yet running under Linux. I gratefully acknowledge financial support from the "Fonds der Chemischen Industrie".

## C++ program Y290

The source code of program Y290 consists of a file with the main event-loop: main.cpp and, at the moment, (version: 1.09) further 42 files, all with ending: \*.cpp and corresponding header-files, ending with: \*.h. The makefile is important for compiling and linking all source-files to an executable module. Program Y290 uses shared libraries and has, at the moment, a size of 480K.

The advantages of the Linux system are: 1.) multi-user and multi-tasking facilities, 2.) network-availability, 3.) network-transparency, 4.) stability of the system and 5.) excellent debugging techniques.

In Fig. 2 the startscreen of program Y290 is shown. Fig. 3 shows a screenshot during centering of one reflection and, finally Fig. 4 shows the program during the data collection.

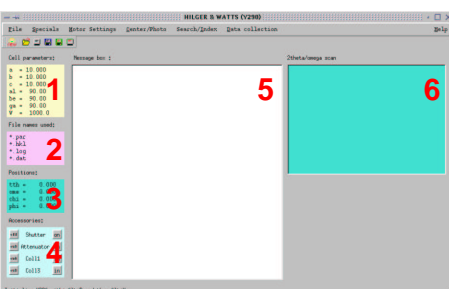


Fig. 2: Screenshot of program Y290 [7] just after the start of the program. At first the serial line (RS232) has to be initialize, then the interface. The program is menu-driven and easy to use.