

# PMATCHC: A Program to MAnage ThermoCHemical data, written in C++

(Version 1.1, 31-08-2001)

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Software Distribution Package (Web); Version 15-09-2002

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The compressed archives **PmatchCW\_a.exe** (Windows) and **PmatchCL.tar.gz** (Linux) contain the distribution package for version 1.1, 31-08-2001, of PMATCHC, a Program to MAnage ThermoCHemical data written in C++. This version of PMATCHC is available for both MS Windows and Linux operating systems. The source code for both versions is the same and requires compilation together with the Qt Toolkit, version 2.0 or higher (© Troll Tech AS, Norway). This toolkit was chosen because it allows PMATCHC to be used either under Linux or Win32 platforms. The Qt Toolkit (GNU licence for Linux, commercial licence #1435740 for Windows) was used to program the PMATCHC code in C++. Borland C++ Builder 5 (standard) was used for compiling the Win32 version and GNU C++ (gcc, egcs) for compiling the Linux version.

## DOCUMENTATION:

The program and its use are described in Paul Scherrer Institut, Waste Management Laboratory Report TM-44-01-07 (**TM-44-01-07.pdf**). A discussion of data generation problems that can arise when PMATCHC is run with certain incomplete data sets is given in Paul Scherrer Institut, Waste Management Laboratory Report AN-44-01-23 (**AN-44-01-23.pdf**). Known problems of the current version of PMATCHC are listed in the file **Problems.pdf**.

## ARCHIVE WINDOWS VERSION:

Files for the Windows version are contained in the self-extracting zip file **PmatchCW\_a.exe**. This will create the directory **\PmatchCW\** in a location of the user's choice, with the following structure:

```
PmatchCW
|
|--BacFile
|--Database
|--Scripts
|--Phrqc_Scripts
|--Program
|   |--bmp
|   |--doc
|   |--HTML
|--Src
|   |--bmp
|   |--core
|   |--doc
|   |--libs
|   |--windows
|       |--Dlg
```

## Subdirectory **\Program\**

This directory includes the file **pmatchc.exe**, the Windows-executable version of the program. It also includes files **cc3520.dll** and **imm32.dll**, which are required to run **pmatchc.exe** in Windows 95, 98 and NT. The file **imm32.dll** should be deleted if **pmatchc.exe** is run under Windows 2000.

Subdirectory **\Program\** also contains two further subdirectories, **\bmp\** and **\doc\**. **\bmp\** includes bitmaps used in PMATCHC windows. **\doc\** contains subdirectory **\html\**, which includes help files in html format that are called from PMATCH. Note that in this release of the program these files are merely place holders. For program help, the user should refer to the documentation (**TM-44-01-07.pdf**).

## Subdirectory **\Src\**

This directory contains the source code for PMATCHC in subdirectories **\core\**, **\libs\** and **\windows\**. It includes subdirectory **\doc\** and a second copy of subdirectory **\bmp\**, which is also in **\Program\**.

Subdirectory **\doc\** contains text files for the license for the QT package, a notice to code users and file **PMATCHC-source-guide.html**, which describes the source code modules.

Directory **\src\** also includes the makefiles which contain the commands to compile and link PMATCHC with either version 4 or 5 of Borland C++ builder and version 2.2.x of QT library.

## Subdirectories **\Database\** and **\Bacfile\**

These subdirectories contain the files for the Nagra/PSI Chemical Thermodynamic Data Base 01/01.

Subdirectory **\Database\** contains the binary data base files (documentation section 5.2) and subdirectory **\Bacfile\** the corresponding backup file **NAPSI\_290502w.BAC** (documentation section 4.1). The subdirectory **\Bacfile\** also contains the file **NAPSI\_290502w\_REF.pdf**, which lists the references for the data base files.

## Subdirectories **\Scripts\** and **\Phrqc\_Scripts\**

These subdirectories contain example script files for formatting and writing output from PMATCHC (documentation section 4.2).

Subdirectory **\Scripts\** contains several relatively simple script files for writing various data tables. The use of these script files is explained in **Scripts.pdf**.

Subdirectory **\Phrqc\_Scripts\** contains the script files needed to write a PHREEQC data file from PMATCHC. These scripts are described in the file **PhreeqcScripts.pdf**.

## **ARCHIVE LINUX VERSION:**

Files for the Linux version of PMATCHC are contained in file **PmatchCL.tar.gz**. When expanded, this file produces directory **\PmatchCL\**. The structure and contents of this directory are virtually the same as those of the Windows version. Because of the variety of Linux flavours that are in use, an executable version of PMATCHC is not included. Each user should compile the program on his or her system.

This code can be compiled on systems running in KDE Workstation mode on which QT.devel... rpm and XFree.86.devel... are installed. After **PmatchCL.tar.gz** has been unpacked, PMATCHC can be compiled by entering "make".