



Indexar patrones de difracción

- Es posible indexar un patrón de difracción de polvo haciendo uso de software gratuito disponible en la red (internet).
- Por ejemplo, para realizar los ejercicios de indexación de patrones de difracción de polvo siguientes, necesitamos en nuestra computadora cargar el software gratuito disponible en los enlaces que se refieren a continuación:



1. El programa WinPLOTR

- <http://www.cdifx.univ-rennes1.fr/winplotr/winplotr.htm>
'winplotr_package.zip'

WinPLOTR - Mozilla Firefox

Archivo Editar Ver Historial Marcadores Herramientas Ayuda

WinPLOTR

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WinPLOTR

WinPLOTR is a software to plot powder diffraction patterns and can be used as a Graphical User Interface for several programs used frequently in powder diffraction data analysis (ex: FullProf, DicVOL, SuperCELL ...). WinPLOTR has been developed to run on PC's with a 32-bit MicroSoft Windows operating system. WinPLOTR supports Windows 9x (x=5,8), Windows NT versions 3.51 and up, XP and Vista. WinPLOTR software has been build up with Lahey Fortran 90 v4.0, using the Windows facilities of RealWin.

HOW TO INSTALL WinPLOTR on YOUR PC?

- > Download the 'winplotr_package.zip' file on your PC (in the 'c:\temp' directory for example)
- > Unzip the WinPLOTR file
The following files will be expanded in the current directory:

readme.txt:	this file
install.exe:	WinPLOTR install program
winplotr.exe:	WinPLOTR executable file
winplotr.set:	WinPLOTR settings file

WinPLOTR - Mozilla Firefox Avril 2009

Tarea de Difracción ... PowBase - search e... WinPLOTR - Mozilla... Difracción de rayos ... ES 11:58

2. El programa MacMaille-v4

○ <http://www.cristal.org/McMaille/short-manual.html>

'McMaille-v4.zip'



McMaille - program for powder pattern indexing - Mozilla Firefox

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www.cristal.org/McMaille/short-manual.html

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McMaille v4.00

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[Input](#)
[Output](#)
[Strategy](#)

Short Manual - Black Box Mode

McMaille is a program for indexing powder patterns by Monte Carlo and grid search (maille in french = cell in english). The necessary data file is quite simple in automated black box mode :

Download

McMaille version 4.00 is distributed under the GNU Public Licence conditions.

The zipped package contains the executable for Windows 95/98/NT/XP, as well as the FORTRAN source codes (quite short and documented) for both the single and the multi processor machines, and some examples described below.

Get it : [McMaille-v4.zip](#)

The compiler used for building the executable was Intel Visual Fortran 9.1. The parallelized version is realized by using [OpenMP](#) directives.

The package MvMaille-V4.zip contains mainly :

McMaille.exe	: executable for MS Windows, single processor
McMaille.for	: the FORTRAN source code
license.html	: the GNU Public License (GPL)

Tarea de Difracción ... PowBase - search e... McMaille - program... Difracción de rayos ... Descargas ES 12:06

- El documento guía para realizar los ejercicios se encuentra en el blog:

<http:// analisisinstrumentalfisico.wordpress.com/2014/03/>

Abrir el documento: *Indexing-XRD.docx*

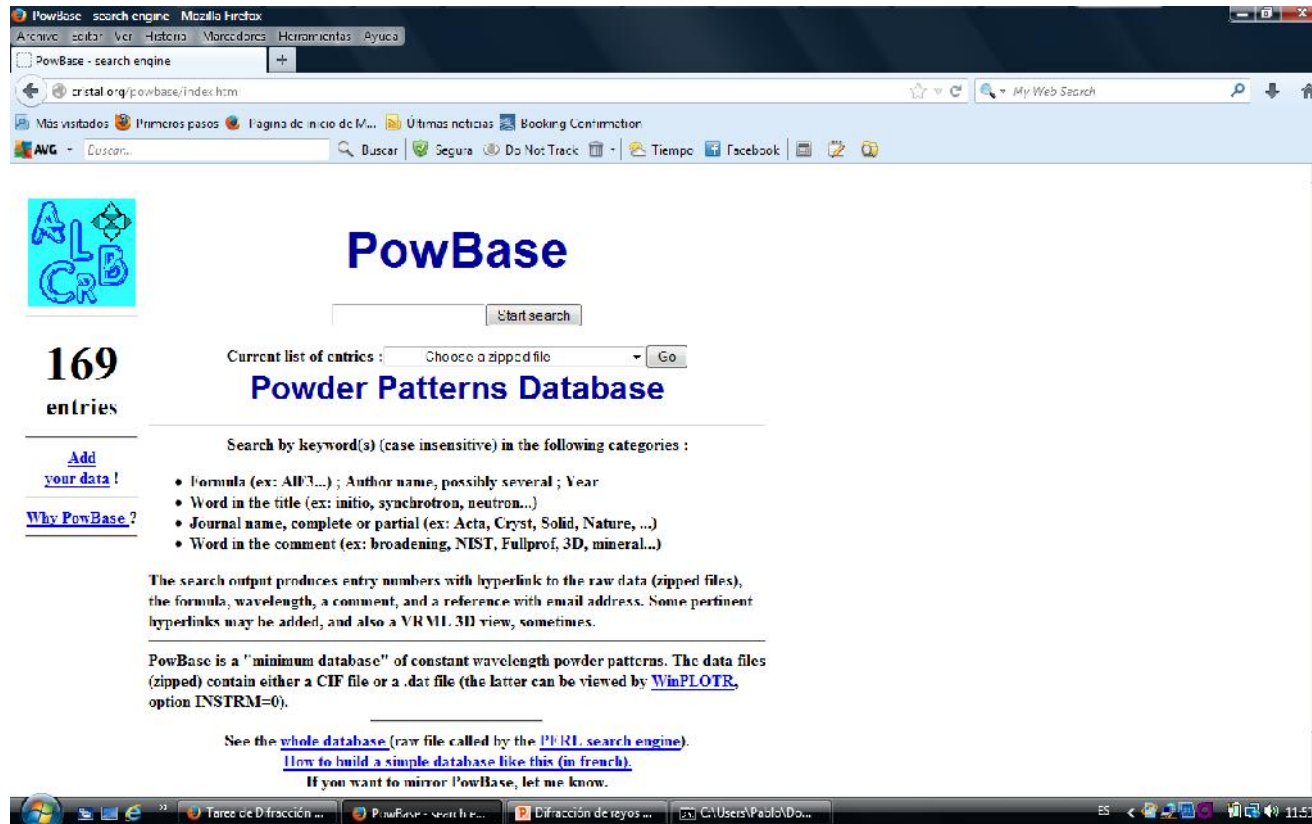
Seguir las instrucciones paso a paso hasta obtener resultados similares a los del ejercicio del óxido de itrio descrito en dicha guía.



- Los difractogramas o patrones de difracción de los ejercicios a realizar se encuentran disponibles en este enlace:

<http://cristal.org/powbase/index.html>

- Powbase es una base datos pequeña de patrones de difracción de polvo.



PowBase - search engine - Mozilla Firefox

Archivos Editar Ver Historial Marcadores Herramientas Ayuda

PowBase - search engine

cristal.org/powbase/index.htm

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ALB
CRB

PowBase

Start search

Current list of entries : Choose a zipcd file Go

Powder Patterns Database

Search by keyword(s) (case insensitive) in the following categories :

- Formula (ex: AlF₃...); Author name, possibly several; Year
- Word in the title (ex: initio, synchrotron, neutron...)
- Journal name, complete or partial (ex: Acta, Cryst, Solid, Nature, ...)
- Word in the comment (ex: broadening, NIST, Fullprof, 3D, mineral...)

The search output produces entry numbers with hyperlink to the raw data (zipped files), the formula, wavelength, a comment, and a reference with email address. Some pertinent hyperlinks may be added, and also a VRML 3D view, sometimes.

PowBase is a "minimum database" of constant wavelength powder patterns. The data files (zipped) contain either a CIF file or a .dat file (the latter can be viewed by [WinPLOT](#), option INSTRM=0).

See the [whole database](#) (raw file called by the [PREFL search engine](#)).

[How to build a simple database like this \(in french\)](#).

If you want to mirror PowBase, let me know.

Tarea de Difracción... PowBase - search... Difracción de rayos... C:\Users\Paola\Do...

ES < > 11:57

- Seleccionar el compuesto número 81, es decir, Y2O3

The screenshot shows a Mozilla Firefox browser window displaying the PowBase website. The address bar shows the URL `cristal.org/powbase/index.html`. The website header features the PowBase logo and a search bar with a "Start search" button. Below the search bar, the current list of entries is shown as "81-Y2O3". A search filter dropdown is set to "Powder".

On the left side of the page, there is a sidebar with the text "169 entries" and a link "Add your data!". Below this, there is a section titled "Search by keyword(s)" with a list of search criteria:

- Formula (ex: AlF3...); Autho
- Word in the title (ex: inicio, s
- Journal name, complete or p
- Word in the comment (ex: br

Below the search criteria, there is a paragraph: "The search output produces entry the formula, wavelength, a comme hyperlinks may be added, and also".

Further down, it says: "PowBase is a 'minimum database (zipped) contain either a CIF file o option INSTRM=0).".

At the bottom of the page, there are links: "See the [whole database](#) (raw file called by the [PERL search engine](#)).", "[How to build a simple database like this \(in french\)](#)", and "If you want to mirror PowBase, let me know."

Overlaid on the website is a file dialog box titled "Abriendo 81.zip". The dialog shows the selected file "81.zip" (21,3 KB) from "http://cristal.org". It asks "¿Qué debería hacer Firefox con este archivo?" and offers two options: "Abrir con WinRAR archiver (predeterminada)" and "Guardar archivo". The "Guardar archivo" option is selected. There are "Aceptar" and "Cancelar" buttons at the bottom of the dialog.

The Windows taskbar at the bottom shows several open applications: "Tarea de Difracción...", "PowBase - search e...", "Difracción de rayos...", and "C:\Users\Pablo\Do...". The system clock shows the time as 11:55.