

Kcrystal: Linux 'live-CD' for powder crystallography

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1. Introduction

We wish to present a distribution of the GNU/Linux (Stallman & GNU team, 1984; Torvalds & Kernel team, 1991) operating system (OS), called *Kcrystal*, the main merit of which is to bring together and distribute crystallographic software in a simplified way. *Kcrystal* is a Linux 'live-CD' (a Linux system running from a bootable CD) that contains a collection of the main software (free distribution) used in the Rietveld method. It was configured to be an easy-to-use tool besides allowing the development of crystallographic software.

The installation and configuration of the Linux OS is often difficult for beginners, as this kind of software requires a degree of effort to become accustomed to. For a user who is unfamiliar with Linux, it can prove to be a difficult platform to use as a work tool on a day-to-day basis.

In order to make Linux more accessible and to provide an easy-to-use tool incorporating crystallographic software developed on this platform, the *Kcrystal* live-CD was created. The programs contained on the live-CD were configured in such a way as to allow the initialization of the operating system directly from the CD drive, without the need to use the operating system installed on the computer hard drive. The user also can opt to install the package on the HD. In both cases, the identification of the hardware and the configuration of the software are automatic.

2. Description

Kcrystal is currently configured with a collection of software that is mainly utilized for crystallography. To use it, it is necessary for the computer to be PC compatible, with a minimum of 128 MB of RAM and a bootable CD drive. The installation on the HD requires a 1.5 GB partition.

The programs are available for immediate use with manuals and internet links to the Web pages of the respective authors. *Kcrystal* uses the Kurumin (Morimoto & Kurumin team, 2003) operating system as its execution platform, a Brazilian descendent of Knoppix/Debian

(Knopper & Knoppix team, 2004; Murdock & Debian team, 1993), currently configured to the Portuguese and English languages.

In the current version, the following Rietveld software is included: *GSAS* (Larson & Von Dreele, 1986), *FullProf* (Rodrigues-Carvajal, 1990) and *RIETAN* (Izumi & Ikeda, 2000) for the Rietveld method (Rietveld, 1969), and *MAUD* (Lutterotti *et al.*, 1999) for pole figures and texture analysis. From a user's perspective, the differences among these three programs are in the mode of execution. The preference for one or another depends on the user. For *GSAS* and *FullProf*, there are user-friendly interfaces, *EXPGUI* (Toby, 2001) and *Winplor*, respectively, helping the user to manage the work. For *RIETAN*, the input control file is very complicated, and the user needs to be very careful while managing it. *RIETAN*, combined with the program *MEED* (Sakata *et al.*, 1990; Kumazawa *et al.*, 1993), can be used for the maximum entropy method (Sakata & Sato, 1990; Collins, 1982).

With *GSAS*, the *EXPGUI* graphical interface and the *PATE*, *COUE* and *FOUE* (Belmonte, 2002) tools for conversion of files to Fourier map, ASCII and Bruker *Topas* formats are included. Profile shape adjustment can be performed using the *Fityk* (Wojdyr, 2004) software. To verify the CIF (Hall *et al.*, 1991) archive syntax, the software *VCIF* (McMahon, 1998) is included. Structure determination can be facilitated using *ITO* (Visser, 1969), *DICVOL* (Boultif & Lower, 1991) or *TREOR* (Werner *et al.*, 1985) software, the source code of which has been adapted for use with *Kcrystal*. As suggested above, *MEED* software is also available for the maximum entropy method.

GNU Fortran, C, C++ and Pascal compilers are available with a great number of supporting libraries, not to mention TCL, TK, wxWin, FFTW, BLAS, GSL (GSL team, 1996) and ObjectCrys++ (Favre-Nicolin, 2001), which are in common use in crystallographic software. The graphics environment chosen was KDE (Ettrich & KDE team, 1997), with text editors, electronic spreadsheets, web browsers and a vast array of Linux application software. The visualizing of scientific data can be done using *OpenDX* (OpenDX Project, 2004) and also using packages such as *ChemTool* (Volk & Chemtool team, 2001), *GDIS* (Fleming, 2004), *GRI* (Kelley & Galbraith, 2000), *ViewMol* (Hill, 2003), *XDrawChem* (Heger, 2002), *YGraph* (Pollney, 2002) and *Ghemical* (Hassinen & Peräkylä, 2001).

Kcrystal is available as a CD image in ISO format and, at the moment, is hosted by: <http://labcacc.iq.unesp.br/kcrystal> and <http://www.ccp14.ac.uk/ccp/web-mirrors/kcrystal>. *Kcrystal* is free software, which may be redistributed and modified according to the terms of the GNU General Public License (FSF, 2005).

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