CCP14 MANUAL - Version 3.0

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Conditions of Use

PLEASE NOTE :

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CCP14 does not accept responsibility for errors resulting from the use of programs contained in the suite.

Introduction

This document has been written to complement the Third Release of the CCP14 Suite, made on 12th December 1996. The anonymous FTP directory structure has been modified slightly for the Third Release, and the new system is illustrated in **Fig. 1**, showing the storage locations of all of the programs in the suite. The **Table 1**, **Table 2** and **Fig. 1** referred to in the following sections are available as postscript files **table1.ps**, **table2.ps** and **fig1.ps**, together with this document **manual.ps**, in the CCP14 anonymous FTP directory **doc/manual**, (see below).

Accessing the CCP14 Suite

There are two ways of using the CCP14 suite. The first option, only for users with accounts on the Daresbury X-ray diffraction server XRDSV1, is simply to type the executable name, followed by the appropriate input and output filenames, if required. This can be done from any directory within the user's account. Those who wish to use CCP14 in this way should go to their XRDSV1 account and type **ccp14help** for more information. The second alternative is to acquire executables compiled and linked for a variety of operating systems, available via anonymous FTP from CCP14. The availability of programs for distribution in this way is indicated in Table 1 and Table 2.

Distibution by Anonymous FTP

The anonymous FTP account is mounted on GSERV1 at Daresbury. To access it, simply type **ftp gserv1.dl.ac.uk** or **ftp 148.79.80.10** and then insert **anonymous** for the userid, followed by your own e-mail address for the password. Next, type **cd ccp14** to go down to the top level of the distribution tree, which is illustrated in Fig. 1.

Below directory **ccp14** is a set of twelve sub-directories, ten of which contain executables whilst sub-directory **source** contains programs for which CCP14 will distribute only source code, and sub-directory **doc** contains the documentation and example input data files for all of the programs within the CCP14 Suite. Directory **doc** is arranged so that all the documentation and example data files corresponding to any one program are grouped in a sub-directory with the name of that program. Directory **doc** also contains a file **update.txt**, indicating all the updates to the suite, including their dates, since the most recent release. Each of the ten executable sub-directories contains executables compiled and linked to run on the operating system indicated by its name, for example **sgirix5.2**. The directory structure below **sgirix5.2** is indicated in Fig. 1, and is identical to that below the other executable directories. Essentially, the executable programs are grouped according to their respective functions, ie. :

* **PEAKF** - Peak searching and fitting software; **fit**, **fourya**, **pkfit**, **shadow** and **xfit**.
* **INDEX** - The autoindexing programs **ito**, **dicvol91** and **treor90**, together with the linking program **indexinp** to set up the input data files for these three indexing programs.
* **CELSYM** - The **testsym** and **tracer** cell symmetry testing programs and the **lapod** program for cell parameter refinement.
* **DECOMP** - Profile decomposition software; **mprep5** and **mprofil5**.
* **PROFIL** - The **profil** suite.
* **FULLPROF** - The **fullprof** suite.
* **GSAS** - The **gsas** suite.
* **MOTPLOT** - The **motplot** spectrum handling package.
* **QUANT** - The **nbs*quant85** quantitative analysis package.

* **STRUC** - The structure solution and display packages **powder cell**, **sirpow**, **struvir**, **psplot**, **ortep3** and **shelin**.
* **SOURCE** - The installation-dependent source code for the DIFRAC system of routines for processing raw diffractometer data into a standardised form.

The CCP14 Suite

There follows a listing of the CCP14 programs, including a brief summary of the operation of each, a statement of the required command line and instructions on where to find help and documentation. On behalf of the academic community, the CCP14 secretary wishes to thank all the program authors who have contributed their software to the suite.

* **FIT** - by V. Petkov and N. Bakaltchev.
A peak-fitting program specifically designed to run on a PC with a built-in graphics facility. The command line is **fit** *input filename*, whereupon menu mode is activated and the user should strictly follow the steps in the upper right (menu) window. Different options in the menu window are selected by means of the arrow keys, and activated by pressing **RETURN**. The options include profile smoothing, background correction, peak-searching and peak-fitting. The user can exit the program at any time with the command **CTRL Q**. Full documentation is contained in the file **fit.doc**, together with an example input data file **cho**, in the FTP directory **doc/fit**.

* **FOURYA** - by A. A. Coelho and R. W. Cheary.
An interactive and graphical X-ray Line Profile Fourier Analysis program, which has been developed to run from an MS-Windows environment. The program performs deconvolution of a reference X-ray diffraction profile and a broadened X-ray diffraction profile in real time. **fourya** is run by means of the MS-Windows **run** command. From the program manager window, press the **file** button and select the **run** option. Then, in the window box provided, type *****/fourya.exe**, where ******* is the directory path to the executable fourya.exe. Immediately, the main control window will appear, entitled **Line Profile Fourier Analysis**. To initiate execution, press the **file** button and select the **load data** option to allow input of data to the program. Full documentation, as a Microsoft Word document **fourya.doc**,

and example input files are available in the documentation directory **doc/fourya**.

*** PKFIT** - by A. D. Murray and A. N. Fitch.

A program which fits a given peak within a powder diffraction profile, for example. The user is prompted for various parameters, including peak shape function, background function and approximate peak position. The program works on a Daresbury *.pds* file and should be used from within the same directory as the appropriate *.pds* file. The result is a statement of the quality of fit and the calculated 2θ value of the peak, which can then be used for indexing. The **command line** is simply the executable name **pkfit**. The associated help file **pkfit.doc** can be obtained from the FTP directory **doc/pkfit**, together with an example *.pds* file **cim.pds**.

*** SHADOW** - by S. A. Howard.

A general pattern analysis program, whose features include peak-searching and peak-fitting by refinement of peak parameters. N.B. The graphics package associated with **SHADOW** has not yet been incorporated into CCP14, but it is intended to make this addition as soon as possible. The command line is simply **shadow**, or **run shadow** from a VMS system, and the user is prompted for all necessary information. Full documentation is contained in the file **shadow.doc** which is located in the FTP directory **doc/shadow**, together with a number of example *.xda* input files.

*** XFIT** - by A. A. Coelho and R. W. Cheary.

An interactive and graphical X-ray Line Profile Fitting package which has been developed in conjunction with **fourya** (see above) to run from an MS-Windows environment. **xfit** integrates the familiar Pseudo Voigt and Split Pearson functions with a Fundamental Parameters approach to generating line profiles. This strategy allows the synthesis of a calculated X-ray diffraction pattern from any number of peaks of any type. **xfit** is run by means of the MS-Windows **run** command. From the program manager window, press the **file** button and select the **run** option. Then, in the window box provided, type *****/xfit.exe**, where ******* is the directory path to the executable xfit.exe. Immediately, the main control window will appear, entitled **X-ray Line Profile Analysis**. To initiate execution, press the **file** button and select the **load data** option to allow input of data to the program. Full documentation, as a Microsoft Word document **xfit.doc**, and example input files are available in the documentation directory **doc/xfit**.

*** INDEXINP** - By A. J. Holland.

An interactive program to generate automatically the input data files for the indexing programs **DICVOL**, **ITO** and **TREOR**. 2theta(d-spacing) values may be entered either interactively or via a special file whose name can be chosen by the user, and which should contain one 2theta(d-spacing) entry per line and nothing else. If the user chooses this option, then it is best to generate the file before running **INDEXINP**. However, if this has not been done, then there is an opportunity within **INDEXINP** to exit program and create the file before returning to **INDEXINP**. The command is simply **indexinp** from UNIX and PC, or **run indexinp** from VMS. The program prompts the user for all necessary data, and then generates the three files **dicvol91.inp**, **ito.inp** and **treor90.inp**, which can be used directly with **DICVOL91**, **ITO** anf **TREOR90**. Full documentation is available in the file **indexinp.doc** in the FTP directory **doc/indexinp**, which also contains an example 2theta(d-spacing) entry file, **cim.dat**, corresponding to the cimetidine data set.

* **DICVOL91** - by D. Louër.
A third alternative for autoindexing, which performs the same function as the two previous programs, by means of the method of *successive dichotomy*. This time, the data from the input file should be explicitly fed into the executable, and the results of the calculations should be fed explicitly into a suitably named output file. On UNIX systems this can be done by *piping* the input and output data, in which case the **command line** is, for example:

dicvol ⟨dicvol91.inp ⟩dicvol91.out

An example input data file, **dicvol91.inp**, together with the full documentation file **dicvol91.doc**, is given in FTP directory **doc/dicvol91**. On VAX systems, input and output is handled by means of a file **dicvol.com**, which can be obtained from the anonymous FTP directory **doc/dicvol91**. The command line is then simply **@dicvol**, and the program will prompt for the names of the input and output files.

* **ITO** - by J. W. Visser.
The program takes a series of 2θ values corresponding to the peaks in a powder diffraction experiment and calculates the reflection indices of each peak, together with the lattice parameters of the unit cell. The **command line** is simply **ito** on a UNIX machine or **run ito** on VMS, since input is taken by default from the file **ITOINP.DAT** and output is written by default to the files **ITOUT.LST** and **ITOSUM.LST**. The associated help file **ito.doc** can be obtained from the FTP directory **doc/ito**, together with an example input file **ITOINP.DAT**.

* **TREOR90** - by P. E. Werner.
Another autoindexing program, which performs the same function as **ITO**. The **command line** is simply **treor** on a UNIX system or **run treor** on a VMS system, upon which the program prompts the user for the names of the input file, the output file, and a condensed output file. If a satisfactory solution is found, then the con-

densed file will contain all relevant information, including a list of indexed reflections. However, in some difficult cases, the general output file contains extra information which may be useful. The user should choose a name for each data set and then call the input, output and condensed files **name.inp**, **name.out** and **name.con**, respectively. An example input file, **treor90.inp**, together with the documentation file, **treor90.doc**, is to be found in the FTP directory **doc/treor90**.

* **LAPOD** - by J. I. Langford.

A program to perform least-squares refinement of cell dimensions from powder data by Cohen's Method.

The command line is simply **lapod** from UNIX or PC, and **run lapod** from VMS.

Input:

Input data via **filename.lap** for UNIX and VMS and **filename.LAP** for PC version. For UNIX and VMS versions, only type the filename, since the extension is added by the program. For the PC version, type the full file designation, including the *.LAP* extension. An example is **baf2.lap**, located in the FTP directory **doc/lapod**.

Output:

Output is sent to **filename.out** for UNIX and VMS, and **filename.OUT** for PC version. For UNIX and VMS versions, only type the filename, since the *.OUT* extension is added by the program. For the PC version, type the full file designation, including the *.OUT* extension.

Full documentation of the program is available in file **lapod.doc** in the FTP directory **doc/lapod**.

* **TESTSYM** - by A. Rulmont.

A program to test the proposed symmetry of the unit cell, given space group etc.

The required input is a file of the same format as **caso3.dat**, **licu.dat**, **nascte.dat** or **rbscte.dat**, which can be found in the FTP directory **doc/testsym**. The name of the input file is entirely the choice of the user. Having thus created the input file, the user should simply type **testsym**, or **run testsym** on VMS, to invoke the program, which will prompt for the name of the input file and the name of the file into which output is to be sent. The results of **TESTSYM** on the input files quoted above are, respectively, **caso3.res**, **licu.res**, **nascte.res** and **rbscte.res** and can be found, along with the full documentation file **testsym.doc**, in the FTP directory **doc/testsym**.

* **TRACER** - by S. L. Lawton.
A program to perform lattice transformation and cell reduction.

To invoke the program, simply type **tracer** from a UNIX or PC system, or **run tracer** from VMS. Then, please insert the name of the input file and the name you wish to give to the output file, when you are prompted. The filename qualifier (*.dat*, *.out*, etc.) should be included when the filename is typed in following the corresponding prompt. The full documentation file is **tracer.doc**, located in the FTP directory **doc/tracer**, containing comprehensive details of input file format. Directory **doc/tracer** also contains the example input file **test.dat** whose format is described in the documentation. The result of **TRACER** on **test.dat** is **test.out** in the same directory.

* **MPREP5 and MPROFIL5** - by A. N. Fitch, A. D. Murray and A. Jouanneaux. A pair of programs which act sequentially to perform profile decomposition.

MPREP5 subtracts an estimated background, if desired, and then associates each point in the diffraction profile with a particular reflection. This requires an input file which includes lattice parameters, X-ray wavelength, zero error in 2θ, counts values and their corresponding values of 2θ, as well as a listing of reflection indices with their multiplicities. An example input file, **cim.pre**, can be found in the FTP directory **doc/mprofil5**, together with the documentation file **mprofil5.doc**, which contains definitons of the entries in the input files for both **MPREP5** and **MPROFIL5**. An appropriate **command line** would then be:

mprep5 ⟨cim.pre ⟩mprep.out

MPROFIL5 refines the above profile and extracts the intensities from the data prepared in **MPREP5**. An example input file, **cim.pro**, can be found in the FTP directory **doc/mprofil5**. An appropriate **command line** would then be:

mprofil5 ⟨cim.pro ⟩mprofil.out

*** PROFIL** - by J. K. Cockcroft.

A completely new Rietveld program, capable of simultaneous refinement of both X-ray and neutron data sets. As well as the Rietveld program **PROFIL** itself, there are several related routines, eg. **PREPAR** for generating a preparatory **.pre** file, **PREPRO** for generating the corresponding binary file, and **JACKAL** for plotting the successfully refined structure. The **command line** for each program is simply the executable name, eg. **profil**, **prepar** etc. (in lower case) on UNIX systems, and on VMS systems the executable name preceded by the command **run**. In each case, the user is prompted for all necessary input data. Thorough documentation has been provided by the program author, Dr. J. K. Cockcroft, as a tex file **profil.tex** or postscript file **profil.ps** in the anonymous FTP directory **doc/profil**.
N.B. PROFIL is not available to run on XRDSV1.

*** FULLPROF** - by J. Rodriguez-Carvajal.

A program for whole-profile refinement and fitting of neutron (nuclear and magnetic scattering) or X-ray powder diffraction data collected at constant steps in 2theta. To invoke the program, the user should simply type **fullprof** from UNIX or PC platforms, or **run fullprof** from VMS. The program will then prompt the users for all necessary infomation. Full details are contained in the file **fullprof.doc** which is located, together with a number of example data files, in FTP directory **doc/fullprof**.

*** GSAS** - by A. C. Larson and R. B. Von Dreele.

The *General Structure Analysis System* (GSAS) is a data processing and analysis package for single crystal and powder data, obtained with either X-rays or neutrons. The package contains numerous routines to perform a very wide variety of functions, from calculation of molecular geometry to preparation of data for publication, and from calculation of X-ray anomalous dispersion coefficients to drawing of ball-and-stick models. The GSAS executable kits, available for six different operating systems via CCP14, are in a compressed form for economy of storage. Instructions on how to uncompress the files and install them come with each kit. In addition, there is a general-purpose GSAS manual, containing exercises to familiarise the user with the functions offered by the package, which is available as four separate postscript files, **gsasmanual1.ps** - **gsasmanual4.ps**, from the FTP directory **doc/gsas**.

*** MOTPLOT** - by P. C. Stephenson and K. S. Ackroyd.

MOTPLOT has been developed at Daresbury Laboratory for the processing of powder diffraction profiles, from a user-friendly window-box environment. Various functions are available, including;

* the input and display of one or more profile(s),
* the display of the current x,y-coordinates of the cross cursor,

* the editing of title and axis labels, and
* the blowing up of a selected area of the plot.

The full set of files required to run and support MOTPLOT is available from the anonymous FTP directory **motplot** below each of the executable directories **sgirix5.2**, **sunos4.1.3** and **solaris2.4**, these being the operating systems for which the package is available. First of all, the user should locally create a directory called **motplot**. Below this directory, the user should create five sub-directories named **Help**, **afm**, **app-defaults**, **bin** and **scripts**. Then, from within FTP, the user should locate the directory **motplot** and transfer the contents of the FTP sub-directories

Help, **afm**, **app-defaults**, **bin** and **scripts** to the corresponding newly-created local sub-directories. Having done this, the user should set the environment variable **PATH** so that the motplot **bin** sub-directory comes first in the path list. For example, suppose the user has installed the directory **motplot** locally on an alien UNIX system such that its full directory path is:

/alien/home/base/motplot

Then the environment variable **PATH** would be set using the command:

setenv PATH /alien/home/base/motplot/bin:${PATH}

To run MOTPLOT, simply type **motplot** from the directory containing your profile data file(s) and you will be prompted for all the required information. The MOTPLOT sub-directory **Help** contains a number of help and documentation files, each of which has a name indicative of its subject material. Users are recommended to pay particular attention to the general introduction file **introduction.help**, and also **PlotIntro.help**, which describes the plot widget used in MOTPLOT and **PlotDialog.help**, on how to construct a plot of one or more profiles. In addition, on-line help is available by selecting the **help** option from the main MOTPLOT window.

* **NBS*QUANT85** - by R. L. Snyder and C. R. Hubbard.

A package of programs to take the user through all the stages of quantitative analysis. The package was originally written to handle specifically the *.raw* data files generated by the diffractometer control program **AUTO**, developed at the National Bureau of Standards in the 1980's by R. L. Snyder, C. R. Hubbard and N. Panagiotopoulos. For the format of these *.raw* files, see :

AUTO - A real time diffractometer control system; NBSIR 81-2229 (1981).

The **nbs*quant** package consists of six independent but functionally related programs :

(1). **amorphous** - A program to analyse **AUTO** quantitative analysis files for amorphous content by the *Spiking Method.*

(2). **autopair** - A program to convert an **AUTO** raw data file to a format that **GIGIPLOT** can handle.

(3). **cobrag** - A program to carry out a Copland-Bragg analysis for quantitative analysis by the *Internal Standard Method.*

(4). **quant** - A program to process *.run* files created by **runfil** and executed by **AUTO** for Internal Standard and Intensity Ratio quantitative analysis.

(5). **runfil** - A program to create *.run* files from standard *.raw* files prepared by program **AUTO**, in either Internal Standard or Intensity Ratio mode. The *.run* file is the set of data directing the quantitative analysis of an unknown sample.

(6). **spike** - A program to analyse quantitative analysis files generated by the program **AUTO**, by means of the Spiking Method.

Full details of the six programs are contained in the documentation file **nbsquant85** located in the FTP directory **doc/nbsquant85**. Each of the programs above is invoked simply by typing its name, eg. **runfil** on UNIX or PC, and **run runfil** on VMS. The directory **doc/nbsquant85** also contains files **AP1.TXT** to **AP8.TXT**, each of which is a complete listing of the screen output during a run of one or other of the six programs above. Users are especially recommended to take a look at these eight listings in order to familiarise themselves with the functioning of each program.

*** POWDER CELL** - by W. Kraus and G. Nolze.
A program for the representation and display of crystal structures and the calculation of the corresponding powder pattern. The executable is **pc.exe**, and can be run from MS-DOS simply by typing **pc** from the directory in which the executable is stored. Please see the documentation directory **doc/powdercell** for the ASCII documentation file **readme**, a LATEX version of the manual and numerous example data files.

*** SIRPOW92** - by A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, M. C. Burla, G. Polidori and M. Camalli.

A structure solution and display program which uses the **name.hkl** file generated by **MPROFIL5**, along with a control file **name.sir** and a file **form.dat** which contains atomic scattering factors. Example files **yono.hkl**, **yono.sir** and **form.dat** are available in the FTP directory **doc/sirpow**, together with the documentation file **sirpow.doc**. The **command line**, which should be issued from within an X-terminal window if graphics is required, is then:

sirpow ⟨name.sir ⟩name.out

The effect of this line is to calculate the structure and put it into the output file called **name.out**, while simultaneously generating an image of the structure in a graphics window which is set up for the purpose by **SIRPOW**. After all the cycles of refinement have completed, the solved structure is displayed and the user is given the option of modifying the presentation of the image.

*** STRUVIR** and **PSPLOT** - by A. Le Bail.

A structure display package. **struvir** takes an input **.cel** file, containing the atomic positions, symmetry and space group information of a solved structure and converts it into a VRML (virtual reality modeling language) **.wrl** file for 3D visualisation. **psplot** converts **struvir** output into postscript form, which can be sent to a postscript printer in order to obtain a hard-copy image of the structure. To run the programs from UNIX, type **struvir** and **psplot**, respectively, and from VMS type **run struvir** and **run psplot**. The MS-Windows 95 version is available as a zip file. Unzip this file and click on **struvir.exe** in order to run the executable. Full documentation and example input files are available in the documentation directories **doc/struvir** and **doc/psplot**.

*** ORTEP3** - by M. N. Burnett and C. K. Johnson.

A program for performing crystal structure illustrations. Ball-and-stick type illustrations of publishable quality are produced with either spheres or thermal ellipsoids on the atomic sites. The program can also produce stereoscopic pairs of illustrations to aid the visualisation of complex packing arrangements of atoms and thermal motion patterns. Interatomic distances, bond angles and principal axes of thermal motion are also calculated to aid the structural study. To run from UNIX and MS-DOS, simply type **ortep3** and from VMS type **run ortep3**. To make use of the documentation, please first of all read the file **ortep3.txt** in directory **doc/ortep3**.

*** SHELIN** - by R. O. Gould.
An interactive program to set up the input data for the SHELX structure solution package of George Sheldrick. CCP14 is not in a position to offer SHELX itself for distribution. However, **shelin** provides the user with the input files to lead directly into SHELX as a next step. Academic users may then obtain SHELX free of charge from George Sheldrick. On-line help is available as an option from within SHELIN. To run from UNIX and MS-DOS, simply type **shelin** and from VMS type **run shelin**.

*** DIFRAC** - by H. Flack.
A set of routines to convert raw diffractometer data from a variety of different instruments into a standardised form containing full details of the sample and the measurements performed on it. The routines are installation dependent and are therefore offered as source code, so that users can edit appropriately to suit their own systems. The routines are located in the directory **source/difrac**, below the CCP14 AFTP home directory, and the documentation can be found in directory **doc/difrac**.

Users with accounts on XRDSV1 are reminded that the **PDPL** powder diffraction package is still available, and contains programs to perform numerous useful functions. For information on what is available, users should type **pdhelp** from any directory on XRDSV1.

For further information about any aspect of the CCP14 suite, please contact:

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