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CRYSTALS, Issue 10

This disk set contains the current version of CRYSTALS, which includes the interactive graphics package CAMERON. Because of difficulties with future maintenance, we no longer plan to distribute CAMERON as a stand alone program capable of reading data files from other systems.

Bob Gould in Edinburgh has donated the program SXTOCRY, which will generate a file in CRYSTALS format from SHELX.INS files. This may not work completely for very complex SHELX.INS files, but it is a quick way to get started in CRYSTALS.

Most of the changes in Issue 10 are internal, some small bugs have been removed, some output reduced, and more complete cif files are generated. Many SCRIPTS have been improved, and small new details added in response to user requests. The major changes are in the accompanying note.

The new program RC93 replaces RC85 (which is still included) for processing CAD4 and MACH3 output.

Please note the new references for CRYSTALS and CAMERON, and give them with each structure you publish. In the current difficult financial atmosphere in the UK, employers have begun to count the numbers of citations for work, as well as publications, so we will need clear support from the user community if the work is to continue.

CRYSTALS

Watkin, D.J. Prout, C.K., Carruthers, J.R., Betteridge, P.W. (1996). CRYSTALS Issue 10. Chemical Crystallography Laboratory, University of Oxford, Oxford.

CAMERON

Watkin, D.J. Prout, C.K., Pearce, L.J. (1996). CAMERON, Chemical Crystallography Laboratory, University of Oxford, Oxford.

RC93

Watkin, D.J., Prout, C.K., Lilley, P.M.deQ. (1994), RC93, Chemical Crystallography Laboratory, University of Oxford, Oxford.

Work is currently well in hand for the production of a Macintosh version, and we are experimenting with a full Windows version for Intel based machines. The VAX OPEN VMS

version is available, and there are DEC ALPHA versions in existence. The SG version of CRYSTALS works well, but we need help with the X-LIB version of CAMERON.

We are now experimenting with anonymous ftp. If you are interested in helping, we have a distribution kit sitting in the /pub/crystals directory on

darkstar.xtl.ox.ac.uk

In order to download the software, try something like:

```
:          ftp darkstar.xtl.ox.ac.uk
:login/name?    ftp
:password?      "your E-mail address"
:ftp>    cd /pub/crystals        (to move to the correct directory)
:ftp>    ls                      (to see the contents of the directory)
:ftp>    binary                  (to be sure to get the .exe Ok)
:ftp>    mget *.*                (to get everything)
:ftp>    bye                     (to close down)
```

Read the 'readme.ftp' document since it contains an abbreviated installation procedure.

CRYSTALS-PC

CRYSTALS-PC is the mainframe and Work-station version of CRYSTALS ported to machines running DOS on Intel 386, 486 or Pentium processors. The crystallographic facilities are identical with (or superior to) those available on mainframes. Hardware requirements are a VGA screen, 20 Mb hard disk, 16 Mb ram and a 486DX or Pentium processor.

The code runs under the Salford Software Services memory manager, DBOS, which is distributed by us under licence. DBOS conforms to the Virtual Control Program Interface (VCPI) protocol. It may be incompatible with other memory managers, disk caches, or networking software which use Extended Memory or interrupt vectors carelessly. DBOS is compatible with Microsoft WINDOWS95, and can be run in a DOS-Box

The current version of CRYSTALS-PC is experimental, and so is distributed without charge. When we are reasonably content with it, the University may insist that we charge a nominal fee.

The distribution disks only contain the executables, manuals and essential data. The files are compressed using PKZIP (for which we have paid a distribution licence fee), and are self unpacking. Sources may be available by special arrangement.

INSTALLATION

Phase 1, DBOS for DOS 5.xx, 6.xx or WIN95

The disk containing DBOS is a copy of that provided to us by SSS, and contains information about DBOS. If you are running other memory managers or disk cache software, read the DBOS notes carefully. Note that it is compatible with HIMEM AND EMM386. You can install DBOS as follows:

1) Change to the root directory (e.g. C:)
2) Insert the floppy into the drive (e.g. A:)
3) Type A:INSTALL
4) Put DBOS into the default directory, C:DBOS.DIR
5) Do **not** permit INSTALL to modify your AUTOEXEC.BAT

Phase 2, CRYSTALS etc

The floppy labelled CRYSTALS contains the CRYSTALS program and essential data files. The floppy labelled FOREIGN contains the manuals and 'foreign' programs that we have permission to distribute. From the root directory on your hard disk, issue:

	INSTALLC	floppy_drive	hard_disk
	INSTALLF	floppy_drive	hard_disk

Example:

a:
installc a: c:

or **a:installc a: c:**

Phase 3, creating the running environment.

CRYSTALS can be run under DOS-5, DOS-6 or in the WINDOWS95 DOS-box. In the examples below, the environment variables CRDRIVE and CRROOT are set to C: and \CRYSTALS, but other disks and roots are permitted. Items in **bold are mandatory**, other items are optional and may already exist in your files.

CRYSTALS under WINDOWS 95

The simplest way to run CRYSTALS under WINDOWS95 is either to boot the machine as a DOS machine (edit MSDOS.SYS, a hidden file), to interrupt the load of WIN95 (press F8 during the boot), or open a DOS box from the DOS icon. You will need to set certain things in the following files. It is assumed that your WIN95 operating system is in C:\windows, though it may be somewhere else. The lines marked '>' and high-lighted are mandatory, the other lines are included to enable you to identify where to make the additions. **DO NOT edit autoexec.dos, autoexec.w40, config.dos or config.w40.**

AUTOEXEC.BAT:

```
        @ECHO OFF
        PATH C:\WINDOWS;C:\WINDOWS\COMMAND;C:\DOS;C:\UTIL;
>       rem - the drive with the goodies
>       SET CRDRIVE=C:
>       rem - the root directory
>       SET CRROOT=\CRYSTALS
>       SET CRDBOS=FALSE
>    rem - note carefully the '%'s and ';'s.
>       SET PATH=%path%;%crdrive%%crroot%;c:\dbos.dir;
        LH  C:\WINDOWS\COMMAND\DOSKEY /INSERT
        PROMPT $p$g
        LH  mode con codepage prepare=((850) C:\WINDOWS\COMMAND\ega.cpi)
        LH  mode con codepage select=850
        LH  keyb uk,,C:\WINDOWS\COMMAND\keyboard.sys
```

CONFIG.SYS:

```
        DEVICE=C:\WINDOWS\HIMEM.SYS /TESTMEM:OFF
        DEVICE=C:\WINDOWS\EMM386.EXE NOEMS
        BUFFERS=23,0
        FILES=40
        DOS=UMB
        LASTDRIVE=h
        FCBS=4,0
        DEVICEHIGH =C:\WINDOWS\SETVER.EXE
        DOS=HIGH
>       DEVICEHIGH =C:\WINDOWS\COMMAND\ANSI.SYS
>       DEVICEHIGH =C:\WINDOWS\COMMAND\DISPLAY.SYS CON=(EGA,,1)
>       SHELL=c:\WINDOWS\COMMAND.COM /P /E:2048
        Country=044,850,C:\WINDOWS\COMMAND\country.sys
```

MSDOS.SYS: Note that you may have to use ATTRIB -h -s -r filename to clear the file attributes before you edit this file. Reset them afterwards.

```
        ;FORMAT
        [Paths]
        WinDir=C:\WINDOWS
```

WinBootDir=C:\WINDOWS
HostWinBootDrv=C

[Options]
BootMulti=1
> **BootGUI=0** (Note that this is optional, and forces a I
Network=1
;
;The following lines are required for compatibility with other programs.
;Do not remove them (MSDOS.SYS needs to be >1024 bytes).
;xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxa
(more of same - do not remove)

SYSTEM.INI:

[386Enh]
ebios=*ebios
device=*vshare
device=*dynapage
device=*vcd
device=*vpd
device=*int13
device=*vpowerd
keyboard=*vkd
display=*VDD,*VFLATD
mouse=*vmouse, msmouse.vxd
woafont=dosapp.fon
> **device=C:\DBOS.dir\WDBOS.386**

[NonWindowsApp]
> **CommandEnvSize=2048**

CRYSTALS UNDER DOS

Modify CONFIG.SYS to set the maximum number of buffers and files to be at least the values given below, and use the SHELL command to allocate enough space for environment variables.

```
        device=C:\DOS\himem.sys
        install=C:\DOS\share.exe
try     device=c:\DOS\EMM386.EXE NOEMS X=CF00-DF77 D=64      (if you have clashes with your network)

or      device=c:\dos\emm386.exe 3072 ram
        DOS=HIGH,UMB
        buffers=30
        files=100
        DEVICE=C:\DOS\ANSI.SYS/x                  (to enable screen colour changes)
        SHELL=c:\dos\COMMAND.COM /P /E:2048       (you may need to change this to 4096 if you run
                                                   out of environment space)
```

Next, you must edit AUTOEXEC.BAT. If you are using SMARTDRIVE, load it early on, *e.g.*

```
C:\WINDOWS\SMARTDRV.EXE 1024 512
C:\WINDOWS\SMARTDRV.EXE c >nul
```

If you have an old version of CRYSTALS on the machine, BE SURE TO REMOVE REFERENCES TO CRPROC and DBOS from the PATH instruction. If you are running DOS 5.n, add the following line immediately after the PATH instruction.

```
APPEND /e     {dos5 ONLY, before any APPENDs of your own}
```

At the very bottom of AUTOEXEC.BAT, after network drivers, *etc.* have been loaded, include the following lines. They are on the disk CRYSTALS in the file AUTOEXEC.*BIT*. You will need to edit the high-lighted items if you load the system into other than the default disk and directory.

```
rem set up the CRYSTALS environment
rem - the drive with the goodies
    set crdrive=c:
rem - the root directory
    set crroot=\crystals
    @set crdbos=false
    set path=%path%;%crdrive%%crroot%;c:\DBOS.dir;
choice "Do you want to mount DBOS ?"          NOTE  do NOT load DBOS if you are going to run WINDOWS
    if errorlevel 2 goto nodbos
    @set crdbos=true
    @rem load DBOS
    @call dbosload
:dbostrue
:nodbos0
```

You have to decide whether to load DBOS each time you run CRYSTALS (or CAMERON, SHELXS, SIR88), or whether to load it at boot time, and only unload it when you need to run programs which have their own built in memory managers (eg programs compiled with LAHEY or WATCOM). Keeping it loaded saves time at the start of each application, but unfortunately also uses memory. At boot time, you will be asked if you want to load DBOS. If you reply 'Y', then it is loaded and remains loaded. If you reply 'N', it is specifically loaded and unloaded for each CRYSTALS application.

If you ever need to unload DBOS, type 'DBOSKILL'
If you neet to reload DBOS, type 'DBOSLOAD'

Note that DBOS holds onto some memory, even when applications are not running. Other applications may do the same. If you get the message 'insufficient memory' when you try to run CRYSTALS, use MEM or MSD to try to locate which other applications are holding on to memory.

Phase 4, running the test deck.

BEFORE YOU RUN CRYSTALS, YOU MUST HAVE CHANGED AUTOEXEC AND CONFIG AND REBOOTED

Now change to the directory C:\EXAMPLE and issue:

CRYSTALS

You will be asked if you want to use scripts. Reply NO, and at the CRYSTALS prompt, !, type:

#USE HEXAMPLE.DAT

A test deck will be run, exercising various parts of CRYSTALS. If this is successful, change to the directory NKET and issue:

CRYSTALS

You will be asked if you want to use SCRIPTS, answer YES. You will then be shown a menu. Type HELP if you are curious. Type GENERAL to pass to a sub-script, and then TERMINAL, and then VGA. Choose BACK until you return to the master script, then choose

NEWSTART, then (after giving a title), QUICKSTART. The basic parameters are:

cell	7.533 7.533 15.7802 90 90 90	
S.G.	P 41	
Contents	C 32 H 32 N 4 O 16	(note - uppercase)
Wavelength	1.5418	
Data	FSQ	
Format	(3I4, 2F8.2)	[don't forget the brackets]
Reflection file	NKET.REF	

The tree structure for the menus you have just used is:

```
CONTROL
    GENERAL
        TERMINAL
            VGA
            BACK
        BACK
    NEWSTART
        title
        QUICKSTART
            data items
            (back)
        (back)
    (menu)
```

After this, try following the scripts. If you get in a mess type **DIRECT**. This always returns you to the CRYSTALS prompt. You can restart scripts with #SCRIPT CONTROL.

If you don't like menu mode, the PRIMER shows you how to prepare files for execution. If a file has an error in it, it is possible to edit the file without leaving CRYSTALS, by issuing:

$EDIT filename

In fact, most internal DOS commands are available from within CRYSTALS by issuing $DOSNAME parameters at the CRYSTALS prompt. If you dislike script mode, and want CRYSTALS to start in COMMAND MODE every time, edit the file C:\CRYSTALS\CRYSTALS.SRT to insert a space between # and the SCRIPT CONTROL command in lines near the end of the file ("#'space'text" is treated as a comment.)

Multiple CRYSTALS sessions

In principle, you can run several sessions of CRYSTALS simultaneously in different windows. We do not recommend this, but if you want to experiment, remember that CRYSTALS may want to read some CRYSTALS system files (eg the SCRIPTS, COMMANDS.DSC etc). For these to be accessible by several programs simultaneously, they must be give the **read-only** attribute. Doing this also prevents the files from accidentally being deleted, but it also inhibits Defrag tidying up your disk.

Common Installation Problems

There are few recurring problems, and of these the only common one is 'out of memory', or 'insufficient space'. There are several causes:

1 Something in your PATH enables DOS to find CRYSTALS.EXE before CRYSTALS.BAT. Ensure that the .BAT and E files have been correctly placed, ie in CRYSTALS and CRYSTALS\IMAGES.

2 The tsrs you are running are holding on to too much memory for DBOS to be loaded.

3 Your networking software is trying to use the same interrupts as DBOS

NOTE

You should fill in the enclosed Licence Agreements for CRYSTALS and SIR92, and the SHELXS-86 Registration form if you want a copy of the manual and to be put on George Sheldricks mailing list. There is no fee for SIR88 or SIR92, and the manuals are on the disk.

It is a good idea to E-mail to the program authors as soon as possible, so that they can put you on their list of current users, and so inform you of bugs, changes and updates.

SIR88, SIR92 and SHELXS-86 are distributed by us with their authors permission.

Using CRYSTALS

The PRIMER gives a brief introduction and overview of CRYSTALS, but these notes may get you started.

Each separate structure should be in its own sub-directory, and all work done from within that sub-directory. You will need a diffractometer specific program to generate a reflection file in 'SHELX' format (3Im,2Fn.p), with coefficients I, F or F^2. You will also need the basic crystallographic information as used in the test above. If you have atomic coordinates, they should be in CRYSTALS 'LIST 5' format (see Vol 4 of the manual - if you are moving from SHELX remember to remove the 10's added to fix parameters). If you only have atoms in SHELX format, they can be input into CRYSTALS, but the atom type and serial numbers are lost. The syntax of CRYSTALS lists and commands must be found in the primer or manual. This information may either be typed in directly at the prompt, or can be pre-prepared in a file which CRYSTALS will read on the command '#USE filename'. Alternatively, Scripts exist for the input of most data. Once data has been input, it is stored in the data base, so it is not necessary to re input it for subsequent jobs.

Most of the files generated by CRYSTALS have the name CRFILE, with an extension indicating the use.

CRFILE.DSC	This is the binary data base, which is updated continuously.
CRFILE.LOG	This is a log of all input, including that generated by Scripts. It can be edited and used as subsequent input.
CRFILE.PCH	Ascii files, for use in other system, or for archiving.
CRFILE.LI*	Listing files. Subsequent jobs update the value of *, so that old output is not immediately overwritten. #SET GENERATE OFF inhibits this.
CAMERON.*	Files for communication with the graphics module
SHELXS.*	Files for communication with SHELXS
SIR88.*	Files for communication with SIR88

Common Problems

There are some problems often encountered by new users:

1) *The Scripts get into a tangle.* Usually due to the script writer not making allowance for user error. **Get out of Script mode by typing DIRECT. Re-enter Script mode by typing #SCRIPT CONTROL.**

2) *No reflections are found during QUICKSTART.* Either the filename or the format statement is incorrect. **Check the filename, and that the format statement is enclosed in brackets.**

3) *Structure factor calculations fail with error messages about atoms of type Q.* There are peaks remaining from a Fourier search left in the atom list. **Edit the atom list, either with a script, or directly e.g.**

```
#EDIT
SELECT TYPE NE Q
END
```

4) *DIFABS fails.* Either there are no values for Fc, or no orientation matrix. **Compute structure factors (#SFLS enter, CALC enter, END) or input a matrix (LIST 13, there is a script INLIST13).**

5) *Partially occupied special positions.* The occupation factor given in the atom parameter list, LIST 5, is the 'chemical' occupancy, and so is always unity for a non-disordered site. If the atom is on a special position, the 'crystallographic' occupancy (multiplicity) is computed automatically, and multiplied onto the 'chemical' occupancy. **To force CRYSTALS to use unit crystallographic occupancy (and thus only use the term stored as occupancy in LIST 5), set the UPDATE parameter in LIST 23 to NO. There is a script, INLIST23 to help you). You will then need to take care of all occupation factors manually.**

6) *After exit from CAMERON, the atom parameter list contains hundreds of atoms.* Cameron was exited with a packing diagram on the screen, so that the CAMERON.L5 file contained all the generated atoms. **Issue #USE CAMERON.L5I. This will re-input to CRYSTALS atom list which was initially sent to CAMERON. You can now re-enter CAMERON again if you wish to modify the structure.**

7) *You can only vaguely remember the syntax of a command.* **Look in the PRIMER (chapter 16 & 17), or if you have already started the command type a '?' on the next line, or issue #COMMANDS command_name.**

8) *Read/Write error on unit 1.* Unit 1 is the data base, and you have probably either filled you hard disk, or not enabled automatic disk file extension. **Type #DISK enter, EXTEND SIZE=100 TRIES=100 enter, END.**

Useful Ideas

To get the best out of CRYSTALS you need to work with imagination. Some useful ideas are:

1) Use #SCRIPT PLOT (or #CAMERON enter, END enter, #USE CAMERON.L5) to delete or rename atoms, and to see specific interatomic distances in graphics mode.

2) Use #REGROUP enter, SELECT SEQUENCE=YES enter, to automatically renumber atoms so that adjacent atoms have adjacent serial numbers.

3) Use #COLLECT enter, SELECT TYPE=PEAK enter, to bring new found peaks adjacent to existing atoms.

4) Use #LIST 28 enter, MINIMA RATIO=n enter, to set the threshold ratio for 'unobserved' reflections.

5) Order the atoms in the atom list so that atoms which need to be addressed together are adjacent in the list. You can then use an 'UNTIL' sequence to refer to them.

6) If you have multiple similar fragments (e.g. phenyl groups), number the atoms so that they can easily be addressed in commands with an editor (e.g. c(101) until c(106), c(111) until c(116) etc).

7) If you have lots of phenyl groups, and not much data. Use restraints to permit a valid anisotropic refinement. E.g. for the group P(1)-C(1).....C(6)

```
#LIST 16
# first the geometry - this will enforce pseudo 6 fold symmetry, but you could make it 2 fold.
PLANAR P(1) C(1) UNTIL C(6)
ANGLE 180,.1 = P(1) to C(1) to C(4)
DIST 0,.01 =MEAN C(1) TO C(2) C(2) TO C(3) C(3) TO C(4) C(4) TO C(5) C(5) TO C(6) C(6) TO C(1)
DIST 0,.01 =MEAN C(1) TO C(3) C(2) TO C(4) C(3) TO C(5) C(4) TO C(6) C(5) TO C(1) C(6) TO C(2)
DIST 0,.01 =MEAN C(1) TO C(4) C(2) TO C(5) C(3) TO C(6)
# now bond stretching restraints
VIB 0,.01 = C(1) TO C(2) C(2) TO C(3) C(3) TO C(4) C(4) TO C(5) C(5) TO C(6) C(6) TO C(1)
# now angle flexing restraints
VIB 0,.01 = C(1) TO C(3) C(2) TO C(4) C(3) TO C(5) C(4) TO C(6) C(5) TO C(1) C(6) TO C(2)
VIB 0,.01 = C(1) TO C(4) C(2) TO C(5) C(3) TO C(6)
# so far, we have no restraints on the out-of-plane components of Uij
# set up similarity restraints.
U(ij) 0,.02 = C(1) TO C(2) C(2) TO C(3) C(3) TO C(4) C(4) TO C(5) C(5) TO C(6) C(6) TO C(1)
U(ij) 0,.03 = C(1) TO C(3) C(2) TO C(4) C(3) TO C(5) C(4) TO C(6) C(5) TO C(1) C(6) TO C(2)
VIB 0,.03 = C(1) TO C(4) C(2) TO C(5) C(3) TO C(6)
```

Note that the atom list on each bond restraint also occurs in a vibration restraint and a similarity restraint.
There is a script (on the menu for RESTRAINTS) which will set these up for you. The geometrical rigidity can also be imposed as a constraint (with GROUP in LIST 12), though in this case the group must be idealised before refinement begins (#REGULARISE).

8) Hydrogen atoms. Hydrogen atoms can be found or placed geometrically (#PERHYDRO or #HYDROGEN). They can then be refined freely, or as riding atoms (RIDE, in LIST 12). I prefer NOT to refine them in the least squares (except perhaps

for hydrogens in hydrogen bonds), but to delete them and recompute ideal positions after every 2 or 3 cycles. Put the instructions to delete and create the H atoms in a file, which can be #USEd as required.

9) Refinements of highly correlated parameters or ones ill-defined by the data tend to 'blow up'. Don't try to fix this by refining different parameters in different cycles - this only hides but does not fix the problem. Use shift limiting restraints (in LIST 16). e.g. LIMIT .01 U[ISO]. This will limit the shifts in U[iso] to about .01 per cycle. The effects of successive cycles are cumulative. All parameters can be limited like this. The units are the same as the parameters.

CAMERON

Cameron is the graphics module in CRYSTALS. It produces high quality illustrations suitable for publication. It is also a versatile tool for the manipulation and evaluation of structures. It has its own manual

Molecular and packing diagrams can be produced with CAMERON, showing parts of a diagram as ball-and-stick or as ellipsoids. Bonds can be drawn solid, dotted or tapered. Connections may be made or removed. Labels can be placed automatically or under mouse control, and the point size can be varied. Output is in black&white or colour Postscript or encapsulated post script. If you activate CAMERON via the SCRIPT PLOT, and if you intend to reimport coordinates from the screen model take care that the final diagram is not a packing diagram, otherwise the coordinte list (LIST 5) will contain all the equivalent atoms!

PS2EPS

The eps bounding box computed by CAMERON is sometimes too small, so that the edge of the picture may be missing. This utility reads a CAMERON postscript or encapsulated postscript file and creates an encapsulated postscript file with a better bounding box.

RC85

A program for pre-processing CAD4 output

The unsupported (unsupportable?) program RC85 has been compiled under FTN77 by Lisa Peach and David Kinna. It has been seen to execute to completion, and for NKET the results are the same as those obtained on the VAX.

HOWEVER - the code contained many non standard operations (jumping into DO loops, IF blocks, illegal use of arrays etc). These were standardised, but we are unsure if te code still does what the authors intended.

We will do no more work on RC85, but a similar program is being rewritten from scratch to handle input from a variety of diffractometers.

If you decide to use RC85, you will need to edit the file ATT.DAT to set the attenuation factor for your machine.

RC93

Another program for pre-processing CAD4 output.

This is a re-write of RC85, and is much improved. In particular, it prepares the textual data needed for the submission of a full cif file. You will need to insert the attenuator factor for diffractometer in the attenuator file.

SXTOCRY

The program SXTOCRY, written by Bob gould in Edinburgh University, and may be used to convert a SHELX instruction file to a basic CRYSTALS file.

DIPIN

A small program to pre-process DIP2000 output and ask for the small details which might oterwise be forgotten.

CSD2CRY

A small program written by Bruce Foxman (Brandeis University) to convert Cambridge Crystallographic Data Base output to CRYSTALS format.

The CRYSTALS documentation is currently being revised and updated.

The new documents are as Postscript files, extension .PST. The old documents are as text files (VAX RUNOFF), extension .MEM

The Postscript is formatted for the lesser of European A4 paper and US Letter (8 1/2 x 11).

DLS MEM 05/08/93
TWIN MEM 05/08/93

CAMERON PST 02/05/96 The graphics manual (50 pages)
PRIMER PST 08/10/96 An overview of the program - pre-release (40 pages)
CRYSTALS PST 14/01/97 The CRYSTALS reference manual - pre-release (125 pages)
GUIDE PST 14/01/97 A summary of the features available - not quite finished

We hope to have ASCII and html versions in the future

Substantial changes have been made in the internal handling of reflection data to permit the application of DIFABS to either Fo or Fc, and to enable the use of negative F or F^2 values. The least-squares code has been reorganised and linearised to improve performance, and changes have been made in refelction selection. The cif output has been considerably extended, and CAMERON much improved. The principal changes affecting existing users are:

1 The symmetry list, LIST 2, now stores the crystal class (redundant, but an ACTA required parameter). The class ıtomatically saved if the operators are generated from the symbol (#SPACEGROUP).

```
#LIST 2
...
CRYSTAL CLASS=monoclinic
END
```

2 In all reflection processing modules, the permitted values for the keyword F'S have been changed.

Old: F'S = YES or NO
New: F'S = FO of FSQ

3 In all reflection processing modules, the permitted value for the keyword MEDIUM has been changed.

Old: MEDIUM = M/T (For magnetic tape)
New: MEDIUM = File (for a formatted disk file)

4 Reflection acceptance conditions (List 28). The Directives selecting slices of the reciprocal lattice depending on :ction index conditions has an additional keyword, TYPE.

```
SLICE       P= Q= R= S= T= TYPE= ACCEPT or REJECT
CONDITION   P= Q= R= S= T= TYPE= ACCEPT or REJECT
```

5 In TORSION, PUNCH has been replace by PRINT

6 In PARAMETERS, an additionl parameter gives the number of lines on a page. This can be made very large to :rate unpaginated output.

7 In DIFABS, the additional Directive MODE defines the mode of action.

#DIFABS ACTION= MODE= FO or FC or TRANSFER

The default is Fo (as before). Setting Fc causes the correction to be computed and applied to Fc. This is more hematically sound, (see D.W.J. Cruickshank, Crystallographic Computing 1970, Munksgaard, pp 189), but has the dvantage the a merging R factor (R_{int}) cannot be computed directly, and leads to complications in difference electron density s. A temporary solution is to transfer the correction from Fc to Fo at the end of the refinement inorder to determini R_{int} and the lual electron density.

8 Additions and changes to #EDIT. The changes may cause some annoyance to experienced users, but were intended ve more flexibility to users, and a more consistent syntax.

CHANGES. These involve directives where the user must give an atom or parameter identifier, and a value. viously, the user could not predict if the value had to preceed or follow the identifier. Now, if the type of value (*e.g.* real, integer haracter) cannot be predicted by CRYSTALS until the identifier has been given, then the value follows the identifier, otherwise eceeds it. The advantage of putting the identifiers after the value is that strings of identifiers may be given without reinputting value.

TRANSFORM a*11* a*12* a*13* ... a*33* C(4) C(5) C(7) until C(27)
SHIFT a*1* a*2* a*3* OS(1) C(1) until C(12)
ADD 0.25 FIRST(X) UNTIL LAST FIRST(Z) UNTIL LAST
CHANGE C(1,TYPE) N

NEW FEATURES.
SHIFT shift_vector atom_list. This moves all the atoms in the atom list by the three (fractional) components of shift vector.
DEORTHOGONAL atom_list. This enables you to convert atoms input in the MOLAX orthogonal coordinate em into crystal fractions. *e.g.*

ATOM C 111 X=2.34 Y=4.07 Z=0.0
DEORTHOGONAL C(111)

CENTROID serial atom_list. This generates an atom QC(serial) at the centroid of the atom list, and with U_{ij} ng an ellipsoid which will envelop the atoms.

PERTURB esd parameter_list. This applies perturbation with zero mean and given esd to the specified meters. The esd is in the natural units of the parameter.

9 In CAMERON, the directive INCLUDE/EXCLUDE AREA enables an area of the diagran to be included/excluded rawing a polygon around it with the mouse.

10 The keword 'WEIGHT' in reflection handling has been replaced by 'SQRTW', which better reflets the data stored.

11 The directive 'ENERGY' in LIST 16 has been replaced by 'NONBONDED'

12 The directives TARGET & IDEAL in regularise are equivalent to OLD & NEW.

THE CRYSTALLOGRAPHIC SYSTEM 'CRYSTALS'
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Signed(position)(date)

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Chemical Crystallography Laboratory,
9 Parks Road,
Oxford,
OX1 3PD.

NAG*
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Wilkinson House,
Jordan Hill Road,
Oxford,
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The NAG routines are supplied under special agreement between CCLO and NAG. Users requiring the routines for any other purpose must contact NAG directly.

THE CRYSTALLOGRAPHIC SYSTEM SIR92
LICENCE AGREEMENT

This AGREEMENT is made between:

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representative also of

Dipartimento di Scienze della Terra, Universita' di Perugia,
Ist. di Strutturistica Chimica "G. Giacomello", CNR, Roma

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and

('The INSTITUTIO

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