DIRDIF-96

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a Computer Program System for Crystal Structure Determination by
Patterson Methods and Direct Methods applied to Difference Structure Factors

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Documents. See the DIRDIF.PRIMER for a short write-up of the DIRDIF programs and for detailed information on how to run the DIRDIF system, including an example structure: MONOS.
For the terminal: use the DIRDIF .ORBASE-GALLERY which is a visualization of the molecular fragments present in the file ORBASE. The file ORUSER is a supplement to ORBASE with your own fragments! The documents are collected in the DIRDIF USER'S GUIDE which includes theoretical background (lecture notes) and further information.

When to use DIRDIF for routine structure analysis:

1. For structures with heavy atoms, including P and S	call:	PATTY
2. For structures of molecules with (partly) known geometry		ORIENT

When to use DIRDIF for special problem structures:

3. When ab-initio direct methods gave a misplaced fragment	TRACOR
4. For expansion of a small fragment to the complete structure	PHASEX
5. To solve an enantiomorph or a super- or pseudo-symmetry problem	PHASEX

How to run DIRDIF (CCODE identifies the structure) Change to directory CCODE !?
Input: crystal data and reflection data; some options require atomic coordinates. In automatic mode the structural parameters (atomic coordinates, either user-supplied or found by Patterson methods) are expanded and recycled (calling repeatedly the appropriate programs) to determine the complete structure. Output: an ATOMS file with atomic coordinates.

1. Patterson option PATTY for Heavy Atom Patterson interpretation.
To solve a heavy-atom structure (including S or P in a light atom structure), use PATTY in automatic mode. No input atoms needed. Just enter:
=====> DIRDIF CCODE PATTY

2. Patterson option ORIENT for application of Vector Search methods.
Vector Search methods are used when a (relatively small) part of a structure has known geometry. Prior to running ORIENT, the search model (ATMOD file with fractional or Cartesian coordinates) must be prepared. To verify the format of your prefab ATMOD file, or to retrieve a model from ORBASE (visualised in the ORBASE-GALLERY), and/or to modify the model interactively, enter:
=====> DIRDIF CCODE ORBASE
[both ORUSER and ORBASE are searched, in this order.]
Then, for application of ORIENT in automatic mode (valid input ATMOD file available), enter:
=====> DIRDIF CCODE ORIENT
Procedure: orientation by program ORIENT using Vector Search, positioning by programs TRACOR and TRAVEC, and expansion and recycling by PHASEX, etcetera.

Additional options:
3. Positioning of a misplaced fragment (fractional atomic coordinates given in an ATOMS file):
=====> DIRDIF CCODE TRACOR
4+5. Expansion and recycling of a partial structure (fractional atomic coordinates in ATOMS file):
=====> DIRDIF CCODE PHASEX
In case of problems:
=====> DIRDIF H : Invokes a limited help session.
=====> DIRDIF CCODE : Starts an interactive run.
=====> DIRDIF CCODE PHASEX NORECY : automatic run, but recycling is suppressed!

The filename dictates the contents and the format of the file. File names are represented here (as in all programs) by capitals. Local implementation may change capitals into lower case, and/or concatenate the name to the compound code (e.g. the CRYSIN file may be: 'crysin' or 'monos.crysin' where 'monos' is the CCODE of test structure MONOS).

Reflection data files (options), DIRDIF finds out which one is input:

FREF alias FREFA FREFB FREFC :	formatted reflection data file (F values).
HKL alias SHELX SHELXL :	formatted reflection data file (F or F-squared values).

Crystal data files (options), DIRDIF finds out which one is input:

CRYSIN	primary crystal data
INS alias RES	SHELXL control data files
CIF	The IUCr-ActaCryst CIF file (for crystal data only)

Atomic parameters files (input and/or output):

ATMOD	atomic parameters (fractional or Cartesian coordinates) of a molecular model (fragment) for input to ORIENT. This file can be prepared manually, or by calling ORBASE and retrieving a model from ORBASE/ORUSER . Various procedures overwrite this file but input data are copied/appended to the ATOLD file for back up.
ATOMS	atomic parameters (in fractional coordinates) of the structure or of a part of the structure, either as input or as output. Various programs overwrite the ATOMS file with intermediate or final atomic parameters, but input data are appended to ATOLD.
ATOLD	file with a collection of successively produced and/or used ATOMS files (back up).
XYZN	file with control data and atomic parameters in SHELXL format. The XYZN file is written by NUTS at the end of the recycling procedure. When you rename it to INS the file is ready for input to the SHELXL least squares refinement.
SPF	atomic parameters in PLUTON format (A.Spek) output by program NUTS.

Other DIRDIF files:

LIS1	output file with a summary of results and comments, to be inspected and (optionally) printed.
LIS2	auxiliary output file with more (intermediate) information, only to be inspected when LIS1 did not show the complete structure and you want to figure out what went wrong.
DDLOG	file on which the system keeps some data on the subsequent DIRDIF runs.
CRYSDA	extended crystal data (automatically prepared by program CRYSDA)

Results of DIRDIF

When the structure has been solved correctly the atomic parameters of the structure are written onto the ATOMS file (and/or XYZN/SPF file); one proceeds with this file as input to a refinement program.

If your structure has not come out correctly, the output listing files LIS1 and LIS2 give indications to detect where the solution of the structure (probably) went wrong, and you can set up an appropriate strategy to run DIRDIF again: either with non-default parameters, or with a changed model, or using the second solution of ORIENT or TRACOR, etcetera. As DIRDIF produces a number of intermediate sets of atomic parameters and writes them on the ATOMS file or on the ATOLD file, you can pick up the appropriate atomic parameters set from one of them to rerun part of DIRDIF.

Sometimes the automatic recycling in the expansion part of the procedure (PHASEX/FOUR) does not work properly (f.i. when the cell contents are far off): do inspect the results of the first cycle of PHASEX/FOUR, given on LIS2. (Or rerun DIRDIF without the automatic recycling; the additional calling parameter NORECY suppresses the automatic recycling.)

To change the space group or the contents of the unit cell:
change the CRYSIN file and delete the CRYSDA file.