edtools

Release 1.0.4

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API REFERENCE

Collection of tools for automated processing and clustering of batch 3-dimensional electron diffraction (3D ED) datasets.

The source for this project is available here.

CHAPTER

ONE

INSTALLATION

Install using `pip install edtools`. Installation should take less than 20 seconds on a normal desktop.

Find the latest releases for the versions that have been tested on.

CHAPTER

TWO

OS REQUIREMENT

Windows 10 or newer.

CHAPTER

THREE

SOFTWARE REQUIREMENTS

- Python 3.6+ including `numpy`, `scipy`, `matplotlib`, and `pandas` libraries
- `` `sginfo <https://github.com/rwgk/sginfo>`__ `` or `` `cctbx.python <https://cctbx.github.io/installation.html#installation>`__ `` must be available on the system path for `edtools.make_shelx`
- Access to WSL
- XDS package must be installed properly under WSL

CHAPTER

FOUR

PACKAGE DEPENDENCIES

Check pyproject.toml for the full dependency list and versions.

CHAPTER

FIVE

DOCUMENTATION

See the documentation at https://edtools.readthedocs.io.

CHAPTER

SIX

PIPELINE TOOLS

At any step, run *edtools.xxx -h* for help with possible arguments.

6.1 autoindex.py

Looks for files matching `XDS.INP` in all subdirectories and runs them using `XDS`.

```
In:  XDS.INP
Out: XDS data processing on all files
```

Usage:

```
edtools.autoindex
```

6.2 extract_xds_info.py

Looks files matching `CORRECT.LP` in all subdirectories and extracts unit cell/integration info. Summarizes the unit cells in the excel file `cells.xlsx` and `cells.yaml`. XDS_ASCII.HKL files matching the completeness / CC(1/2) criteria are listed in `filelist.txt`. Optionally, gathers the corresponding `XDS_ASCII.HKL` files in the local directory. The `cells.yaml` file can be used as input for further processing.

```
In:  CORRECT.LP
Out: cells.yaml
     cells.xlsx
     filelist.txt
```

Usage:

```
edtools.extract_xds_info
```

6.3 find_cell.py

This program a cells.yaml file and shows histogram plots with the unit cell parameters. This program mimicks `CELLPARM <http://xds.mpimf-heidelberg.mpg.de/html_doc/cellparm_program.html>`__ and calculates the weighted mean lattice parameters, where the weight is typically the number of observed reflections (defaults to 1.0). For each lattice parameter, the mean is calculated in a given range (default range = median+-2). The range can be changed by dragging the cursor on the histogram plots.

Alternatively, the unit cells can be clustered by giving the `--cluster` command, in which a dendrogram is shown. The cluster cutoff can be selected by clicking in the dendrogram. The clusters will be written to `cells_cluster_#.yaml`.

```
In:  cells.yaml
Out: mean cell parameters
     cells_*.yaml (clustering only)
```

Usage:

```
edtools.find_cell cells.yaml --cluster
```

6.4 make_xscale.py

Prepares an input file `XSCALE.INP` for `XSCALE` and corresponding `XDSCONV.INP` for `XDSCONV`. Takes a `cells.yaml` file or a series of `XDS_ASCII.HKL` files as input, and uses those to generate the `XSCALE.INP` file.

```
In:  cells.yaml / XDS_ASCII.HKL
Out: XSCALE.INP
```

Usage:

```
edtools.make_xscale cells.yaml -c 10.0 20.0 30.0 90.0 90.0 90.0 -s Cmmm
```

6.5 cluster.py

Parses the `XSCALE.LP` file for the correlation coefficients between reflection files to perform hierarchical cluster analysis (Giordano et al., Acta Cryst. (2012). D68, 649–658). The cutoff threshold can be selected by clicking in the dendrogram window. The program will write new `XSCALE.LP` files to subdirectories `cluster_#`, and run `XSCALE` on them, and (if available), pointless.

```
In:  XSCALE.LP
Out: cluster_n/
    filelist.txt
    *_XDS_ASCII.HKL
    XSCALE processing
    Pointless processing
    shelx.hkl
    shelx.ins (optional)
```

Usage:

```
edtools.cluster
```

CHAPTER

SEVEN

HELPER TOOLS

7.1 make_shelx.py

Creates a shelx input file. Requires `sginfo` to be available on the system path to generate the SYMM/LATT cards.

```
In:  cell, space group, composition
Out: shelx.ins
```

Usage:

```
edtools.make_shelx -c 10.0 20.0 30.0 90.0 90.0 90.0 -s Cmmm -m Si180 O360
```

7.2 run_pointless.py

Looks for XDS_ASCII.HKL files specified in the cells.yaml, or on the command line and runs Pointless on them.

```
In:  cells.yaml / XDS_ASCII.HKL
Out: Pointless processing
```

7.3 update_xds.py

Looks files matching `CORRECT.LP` in all subdirectories, and updates the cell parameters / space group as specified.

```
In:  XDS.INP
Out: XDS.INP
```

Usage:

```
edtools.update_xds -c 10.0 20.0 30.0 90.0 90.0 90.0 -s Cmmm
```

7.4 find_rotation_axis.py

Finds the rotation axis and prints out the inputs for several programs (XDS, PETS, DIALS, Instamatic, and RED). Implements the algorithm from Gorelik et al. (Introduction to ADT/ADT3D. In Uniting Electron Crystallography and Powder Diffraction (2012), 337-347). The program reads `XDS.INP` to get information about the wavelength, pixelsize, oscillation angle, and beam center, and `SPOT.XDS` (generated by COLSPOT) for the peak positions. If the `XDS.INP` file is not specified, the program will try to look for it in the current directory.

```
In:  XDS.INP, SPOT.XDS
Out: Rotation axis
```

Usage:

```
edtools.find_rotation_axis [XDS.INP]
```

CHAPTER

EIGHT

DEMO OF USING EDTOOLS TO PROCESS BATCH 3D ELECTRON DIFFRACTION DATASETS

See the demo at https://edtools.readthedocs.io/en/latest/examples/edtools_demo.html.

CHAPTER

NINE

API REFERENCE

9.1 edtools

9.1.1 edtools.autoindex

Functions:

clear_files(path)	Clear LP files
connect(payload)	Try to connect to *instamatic* indexing server
main()	
parse_xds(path[, sequence])	Parse XDS output (CORRECT.LP) and print summary about indexing progress to the screen.
xds_index(path[, sequence, clear, parallel])	Run XDS at given path.

edtools.autoindex.**clear_files**(*path: str*) → None

Clear LP files

edtools.autoindex.**connect**(*payload: str*) → None

Try to connect to *instamatic* indexing server

Parameters

payload (*str*) – Directory where XDS should be run.

edtools.autoindex.**main**()

edtools.autoindex.**parse_xds**(*path: str*, *sequence: int = 0*) → None

Parse XDS output (CORRECT.LP) and print summary about indexing progress to the screen.

Parameters

- **path** (*str*) – Path in which XDS has been run
- **sequence** (*int*) – Sequence number, needed for output and house-keeping

edtools.autoindex.**xds_index**(*path: str*, *sequence: int = 0*, *clear: bool = True*, *parallel: bool = True*) → None

Run XDS at given path.

Parameters

- **path** (*str*) – Run XDS in this directory, expects XDS.INP in this directory
- **sequence** (*int*) – Sequence number, needed for output and house-keeping
- **clear** (*bool*) – Clear some LP files before running XDS

- **parallel** (*bool*) – Call *xds_par* rather than *xds*

9.1.2 edtools.cif_tools

Functions:

add_instrument()	
delete_instrument()	
list_instrument()	
main()	
update_cif(fn[, wavelength, description, ...])	

edtools.cif_tools.**add_instrument**()

edtools.cif_tools.**delete_instrument**()

edtools.cif_tools.**list_instrument**()

edtools.cif_tools.**main**()

edtools.cif_tools.**update_cif**(*fn*, *wavelength=None*, *description=None*, *color=None*, *remove_hkl=None*, *reply=None*, *instrument=None*)

9.1.3 edtools.cluster

Functions:

check_for_pointless()	
clean_params(inp)	
distance_from_dendrogram(z[, distance])	
get_clusters(z[, distance, fns, method, ...])	
get_condensed_distance_matrix(corrmat)	
main()	
parse_xscale_lp(fn)	
parse_xscale_lp_initial([fn])	
run_pointless(filepat[, verbose, i])	
run_xscale(clusters, cell, spgr[, ...])	

edtools.cluster.**check_for_pointless**()

edtools.cluster.**clean_params**(*inp*)

edtools.cluster.**distance_from_dendrogram**(*z*, *distance=None*)

edtools.cluster.**get_clusters**(*z*, *distance=0.5*, *fns=[]*, *method='average'*, *min_size=1*)

edtools.cluster.**get_condensed_distance_matrix**(*corrmat*)

edtools.cluster.**main**()

edtools.cluster.**parse_xscale_lp**(*fn*)

edtools.cluster.**parse_xscale_lp_initial**(*fn='XSCALE.LP'*)

edtools.cluster.**run_pointless**(*filepat*, *verbose=True*, *i=0*)

edtools.cluster.**run_xscale**(*clusters*, *cell*, *spgr*, *resolution=(20.0, 0.8)*, *ioversigma=2*)

9.1.4 edtools.extract_xds_info

Functions:

cells_to_cellparm(ps)	Takes a list of *xds_parser* instances and writes the cell parameters to an instruction file *CELLPARM.INP* for the program *cellparm*.
cells_to_excel(ps[, fn])	Takes a list of *xds_parser* instances and writes the cell parameters to an excel file *cells.xlsx*.
cells_to_yaml(ps[, fn])	
cells_to_yaml_xparm(uc[, fn])	
evaluate_symmetry(ps)	
gather_xds_ascii(ps[, min_completeness, ...])	Takes a list of *xds_parser* instances and gathers the corresponding *XDS_ASCII.HKL* files into the current directory.
lattice_to_space_group(lattice)	
main()	
parse_xparm_for_uc(fn)	

Classes:

xds_parser(filename)	docstring for xds_parser

edtools.extract_xds_info.**cells_to_cellparm**(*ps*)

Takes a list of *xds_parser* instances and writes the cell parameters to an instruction file *CELLPARM.INP* for the program *cellparm*.

edtools.extract_xds_info.**cells_to_excel**(*ps*, *fn='cells.xlsx'*)

Takes a list of *xds_parser* instances and writes the cell parameters to an excel file *cells.xlsx*.

edtools.extract_xds_info.**cells_to_yaml**(*ps*, *fn='cells.yaml'*)

edtools.extract_xds_info.**cells_to_yaml_xparm**(*uc*, *fn='cells_xparm.yaml'*)

edtools.extract_xds_info.**evaluate_symmetry**(*ps*)

edtools.extract_xds_info.**gather_xds_ascii**(*ps*, *min_completeness=10.0*, *min_cchalf=90.0*, *gather=False*)

Takes a list of *xds_parser* instances and gathers the corresponding *XDS_ASCII.HKL* files into the current directory. The data source and numbering scheme is summarized in the file *filelist.txt*.

edtools.extract_xds_info.**lattice_to_space_group**(*lattice*)

edtools.extract_xds_info.**main**()

edtools.extract_xds_info.**parse_xparm_for_uc**(*fn*)

class edtools.extract_xds_info.**xds_parser**(*filename*)

Bases: object

docstring for xds_parser

Methods:

__init__(filename)
cell_as_dict()
cell_info([sequence])
info_header([hline])
integration_info([sequence, outer_shell, ...])
parse()
print_filename()

Attributes:

space_group
unit_cell
volume

__init__(*filename*)

cell_as_dict()

cell_info(*sequence=0*)

static info_header(*hline=True*)

integration_info(*sequence=0*, *outer_shell=True*, *filename=False*)

parse()

print_filename()

property space_group

property unit_cell

property volume

9.1.5 edtools.find_beam_center

Functions:

find_beam_center(img[, sigma, m, kind])	Find the center of the primary beam in the image *img* The position is determined by summing along X/Y directions and finding the position along the two directions independently.
find_peak_max(arr, sigma[, m, w, kind])	Find the index of the pixel corresponding to peak maximum in 1D pattern *arr*.
main()	
read_adsc(fname)	read in the file.
readheader(infile)	read an adsc header.
swap_needed(header)	
translate_image(arr, shift)	Translate an image according to shift.
write_adsc(fname, data[, header])	Write adsc format.

edtools.find_beam_center.**find_beam_center**(*img: ~numpy.ndarray*, *sigma: int = 30*, *m: int = 100*, *kind: int = 3) -> (<class 'float'>, <class 'float'>)*

Find the center of the primary beam in the image *img* The position is determined by summing along X/Y directions and finding the position along the two directions independently.

Uses interpolation by factor *m* to find the coordinates of the pimary beam with subpixel accuracy.

edtools.find_beam_center.**find_peak_max**(*arr: ~numpy.ndarray*, *sigma: int*, *m: int = 50*, *w: int = 10*, *kind: int = 3) -> (<class 'float'>, <class 'float'>)*

Find the index of the pixel corresponding to peak maximum in 1D pattern *arr*.

First, the pattern is smoothed using a gaussian filter with standard deviation *sigma* The initial guess takes the position corresponding to the largest value in the resulting pattern A window of size 2*w+1 around this guess is taken and expanded by factor *m* to to interpolate the pattern to get the peak maximum position with subpixel precision.

edtools.find_beam_center.**main**()

edtools.find_beam_center.**read_adsc**(*fname: str) -> (<built-in function array>, <class 'dict'>)*

read in the file.

edtools.find_beam_center.**readheader**(*infile*)

read an adsc header.

edtools.find_beam_center.**swap_needed**(*header: dict*) → bool

edtools.find_beam_center.**translate_image**(*arr*, *shift: array*) → array

Translate an image according to shift. Shift should be a 2D numpy array

edtools.find_beam_center.**write_adsc**(*fname: str*, *data: array*, *header: dict = {}*)

Write adsc format.

9.1.6 edtools.find_cell

Functions:

cluster_cell(cells[, distance, method, ...])	Perform hierarchical cluster analysis on a list of cells.
d_calculator(cell)	Helper function for *unit_cell_lcv_distance*
distance_from_dendrogram(z[, ylabel, ...])	Takes a linkage object *z* from scipy.cluster.hierarchy.linkage and displays a dendrogram.
find_cell(cells, weights[, binsize])	Opens a plot with 6 subplots in which the cell parameter histogram is displayed.
get_clusters(z, cells[, distance])	
main()	
parse_cellparm(fn)	
put_in_order(cells)	order cell parameters in order to eliminate difference in cell distance because of parameter order
to_radian(cells)	convert all angles in unit cell parameter list to radians cells: the cell parameters that are parsed from cells.yaml as np array
to_sin(cells)	convert all angles in unit cell parameter list to sine cells: the cell parameters that are parsed from cells.yaml as np array
unit_cell_lcv_distance(cell1, cell2)	Implements Linear Cell Volume from Acta Cryst.
volume_difference(cell1, cell2)	Return the absolute difference in volumes between two unit cells
weighted_average(values[, weights])	Returns weighted mean and standard deviation

edtools.find_cell.**cluster_cell**(*cells: list*, *distance: Optional[float] = None*, *method: str = 'average'*, *metric: str = 'euclidean'*, *use_radian: bool = False*, *use_sine: bool = False*)

Perform hierarchical cluster analysis on a list of cells.

method: lcv, volume, euclidean distance: cutoff distance, if it is not given, pop up a dendrogram to

interactively choose a cutoff distance

use_radian: Use radian instead of degrees to downweight difference use_sine: Use sine for unit cell clustering (to disambiguousize the difference in angles)

edtools.find_cell.**d_calculator**(*cell: list*) → tuple

Helper function for *unit_cell_lcv_distance*

edtools.find_cell.**distance_from_dendrogram**(*z*, *ylabel: str = ''*, *initial_distance: Optional[float] = None*) → float

Takes a linkage object *z* from scipy.cluster.hierarchy.linkage and displays a dendrogram. The cutoff distance can be picked interactively, and is returned ylabel: sets the label for the y-axis initial_distance: initial cutoff distsance to display

edtools.find_cell.**find_cell**(*cells*, *weights*, *binsize=0.5*)

Opens a plot with 6 subplots in which the cell parameter histogram is displayed. It will calculate the weighted mean of the unit cell parameters. The ranges can be adjusted by dragging on the plots.

edtools.find_cell.**get_clusters**(*z*, *cells*, *distance=0.5*)

edtools.find_cell.**main**()

edtools.find_cell.**parse_cellparm**(*fn*)

edtools.find_cell.**put_in_order**(*cells*)

order cell parameters in order to eliminate difference in cell distance because of parameter order

edtools.find_cell.**to_radian**(*cells*)

convert all angles in unit cell parameter list to radians cells: the cell parameters that are parsed from cells.yaml as np array

edtools.find_cell.**to_sin**(*cells*)

convert all angles in unit cell parameter list to sine cells: the cell parameters that are parsed from cells.yaml as np array

edtools.find_cell.**unit_cell_lcv_distance**(*cell1: list*, *cell2: list*) → float

Implements Linear Cell Volume from Acta Cryst. (2013). D69, 1617-1632

edtools.find_cell.**volume_difference**(*cell1: list*, *cell2: list*)

Return the absolute difference in volumes between two unit cells

edtools.find_cell.**weighted_average**(*values*, *weights=None*)

Returns weighted mean and standard deviation

9.1.7 edtools.find_rotation_axis

Functions:

cylinder_histo(xyz[, bins])	Take reciprocal lattice vectors in XYZ format and output cylindrical projection.
load_spot_xds(fn, beam_center, osc_angle, ...)	Load the given SPOT.XDS file (*fn*) and return an array with the reciprocal
main()	
make(arr, omega, wavelength)	Prepare xyz (reciprocal space coordinates) from reflection positions/angle (*arr*), which is the list of reflections read from XDS (SPOT.XDS)
make_2d_rotmat(theta)	Take angle in radians, and return 2D rotation matrix
optimize(arr, omega_start[, wavelength, ...])	Optimize the value of omega around the given point.
parse_xds_inp(fn)	Parse the XDS.INP file to find the required numbers for the optimization Looks for wavelength, pixelsize, beam_center, oscillation range
plot_histo(H, xedges, yedges[, title])	Plot the histogram of the cylindrical projection.
random_sample(arr, n)	Select random sample of *n* rows from array
rotation_axis_to_xyz(rotation_axis[, ...])	Convert rotation axis angle to XYZ vector compatible with 'xds', or 'dials' Set invert to 'True' for anti-clockwise rotation
rotation_matrix(axis, theta)	Calculates the rotation matrix around axis of angle theta (radians)
xyz2cyl(arr)	Take a set of reflections in XYZ and convert to polar (cylindrical) coordinates

edtools.find_rotation_axis.**cylinder_histo**(*xyz*, *bins=(1000, 500)*)

Take reciprocal lattice vectors in XYZ format and output cylindrical projection. *Bins* gives the resolution of the 2D histogram.

edtools.find_rotation_axis.**load_spot_xds**(*fn*, *beam_center: [<class 'float'>, <class 'float'>]*, *osc_angle: float*, *pixelsize: float*)

Load the given SPOT.XDS file (*fn*) and return an array with the reciprocal
x, y, and angle for the centroid of each reflection

beam_center: coordinates of the primary beam, read from XDS.INP osc_angle: oscillation_angle (degrees) per frame, will be multiplied by the average frame number

that a reflection appears on (column 3 in *arr*)

pixelsize: defined in px/Ångström

http://xds.mpimf-heidelberg.mpg.de/html_doc/xds_files.html#SPOT.XDS

edtools.find_rotation_axis.**main**()

edtools.find_rotation_axis.**make**(*arr*, *omega: float*, *wavelength: float*)

Prepare xyz (reciprocal space coordinates) from reflection positions/angle (*arr*), which is the list of reflections read from XDS (SPOT.XDS)

omega: rotation axis (degrees), which is defined by the angle between x
(horizontal axis pointing right) and the rotation axis going in clockwise direction

Note that:

1. x<->y are flipped

This is to ensure to match the XDS convention with the one I'm used to

edtools.find_rotation_axis.**make_2d_rotmat**(*theta*)

Take angle in radians, and return 2D rotation matrix

edtools.find_rotation_axis.**optimize**(*arr*, *omega_start: float*, *wavelength=<class 'float'>*, *plusminus: int = 180*, *step: int = 10*, *hist_bins: (<class 'int'>, <class 'int'>) = (1000, 500)*, *plot: bool = False*) → float

Optimize the value of omega around the given point.

omega_start: defines the starting angle step, plusminus: together with omega_start define the range of values to loop over hist_bins: size of the 2d histogram to produce the final phi/theta plot plot: toggle to plot the histogram after each step

edtools.find_rotation_axis.**parse_xds_inp**(*fn*)

Parse the XDS.INP file to find the required numbers for the optimization Looks for wavelength, pixelsize, beam_center, oscillation range

edtools.find_rotation_axis.**plot_histo**(*H*, *xedges*, *yedges*, *title='Histogram'*)

Plot the histogram of the cylindrical projection.

edtools.find_rotation_axis.**random_sample**(*arr*, *n*)

Select random sample of *n* rows from array

edtools.find_rotation_axis.**rotation_axis_to_xyz**(*rotation_axis*, *invert=False*, *setting='xds'*)

Convert rotation axis angle to XYZ vector compatible with 'xds', or 'dials' Set invert to 'True' for anti-clockwise rotation

edtools.find_rotation_axis.**rotation_matrix**(*axis*, *theta*)

Calculates the rotation matrix around axis of angle theta (radians)

edtools.find_rotation_axis.**xyz2cyl**(*arr*)

Take a set of reflections in XYZ and convert to polar (cylindrical) coordinates

9.1.8 edtools.make_shelx

9.1.9 edtools.make_xscale

Functions:

get_xds_ascii_names(lst)	
main()	
parse_xds_ascii(fn)	
write_xdsconv_inp(resolution)	
write_xscale_inp(fns, unit_cell, ...)	

edtools.make_xscale.**get_xds_ascii_names**(*lst*)

edtools.make_xscale.**main**()

edtools.make_xscale.**parse_xds_ascii**(*fn*)

edtools.make_xscale.**write_xdsconv_inp**(*resolution*)

edtools.make_xscale.**write_xscale_inp**(*fns*, *unit_cell*, *space_group*, *resolution*)

9.1.10 edtools.period_table

Classes:

App(parent, *args, **kwargs)	

Functions:

main()	

class edtools.period_table.**App**(*parent*, **args*, ***kwargs*)

Bases: Frame

Methods:

__init__(parent, *args, **kwargs)	Construct a frame widget with the parent MASTER.
info(text)	Return information about the packing options for this widget.
name(text)	

__init__(*parent*, **args*, ***kwargs*)

Construct a frame widget with the parent MASTER.

Valid resource names: background, bd, bg, borderwidth, class, colormap, container, cursor, height, highlightbackground, highlightcolor, highlightthickness, relief, takefocus, visual, width.

info(*text*)

Return information about the packing options for this widget.

name(*text*)

edtools.period_table.**main**()

9.1.11 edtools.reflection_tool

Classes:

GroupReflectionsGUI(parent)	A GUI frame for reflections grouping

Functions:

main()

class edtools.reflection_tool.**GroupReflectionsGUI**(*parent*)

Bases: Labelframe

A GUI frame for reflections grouping

Methods:

__init__(parent)	Construct a Ttk Labelframe with parent master.
calc_structure_factors(structures[, dmin, ...])	Wrapper around f_calc_structure_factors() Takes a structure object in which there is only one strcture
check_I_frame_seq()	
corr_prec()	
exti_corr(value, power, param)	
exti_corr_der(value, power, param)	
f_calc_structure_factors(structure, **kwargs)	Takes cctbx structure and returns f_calc miller array Takes an optional options dictionary with keys: input: **kwargs: 'd_min': minimum d-spacing for structure factor calculation 'algorithm': which algorithm to use ('direct', 'fft', 'automatic') structure: <cctbx.xray.structure.structure object> output: f_calc: <cctbx.miller.array object> with calculated structure factors in the f_calc.data() function
gen_fcalc()	
group_df()	
init_vars()	
lorentz_corr(df)	
open_file()	
point_to_rotation_axis(x, y, center, slope)	
read_cif(f)	
remove_reflection()	
save_file(df)	
save_grouped()	
scaling_factor(value, power)	
scaling_func(value, power)	
split_grouped()	
transform_integrated()	
validate(action, index, value_if_allowed, ...)	
validate_range(action, index, ...)	

__init__(*parent*)

Construct a Ttk Labelframe with parent master.

STANDARD OPTIONS

class, cursor, style, takefocus

WIDGET-SPECIFIC OPTIONS
labelanchor, text, underline, padding, labelwidget, width, height

calc_structure_factors(*structures*, *dmin=1.0*, *table='electron'*, *prefix=''*, *verbose=True*, ***kwargs*)

Wrapper around f_calc_structure_factors() Takes a structure object in which there is only one strcture

dmin can be a dataframe and it will take the minimum dspacing (as specified by col 'd') or a float if combine is specified, function will return a dataframe combined with the given one, otherwise a dictionary of dataframes

prefix is a prefix for the default names fcalc/phases to identify different structures

check_I_frame_seq()

corr_prec()

exti_corr(*value*, *power*, *param*)

exti_corr_der(*value*, *power*, *param*)

f_calc_structure_factors(*structure*, ***kwargs*)

Takes cctbx structure and returns f_calc miller array Takes an optional options dictionary with keys: input:

****kwargs:**
'd_min': minimum d-spacing for structure factor calculation 'algorithm': which algorithm to use ('direct', 'fft', 'automatic')

structure: <cctbx.xray.structure.structure object>

output:

f_calc: <cctbx.miller.array object> with calculated structure factors
in the f_calc.data() function

gen_fcalc()

group_df()

init_vars()

lorentz_corr(*df*)

open_file()

point_to_rotation_axis(*x*, *y*, *center*, *slope*)

read_cif(*f*)

remove_reflection()

save_file(*df*)

save_grouped()

scaling_factor(*value*, *power*)

scaling_func(*value*, *power*)

split_grouped()

transform_integrated()

validate(*action*, *index*, *value_if_allowed*, *prior_value*, *text*, *validation_type*, *trigger_type*, *widget_name*)

validate_range(*action*, *index*, *value_if_allowed*, *prior_value*, *text*, *validation_type*, *trigger_type*, *widget_name*)

edtools.reflection_tool.**main**()

9.1.12 edtools.run_pointless

Functions:

main()	

edtools.run_pointless.**main**()

9.1.13 edtools.scattering_factor

Classes:

FitResult_4p(a0, b0, a1, b1, a2, b2, a3, b3, c)	
FitResult_5p(a0, b0, a1, b1, a2, b2, a3, b3, ...)	
ScatteringFactorGUI(parent)	A GUI frame for scattering factor

Functions:

fit_4_param(s, target[, is_xray, method, ...])	
fit_5_param(s, target[, is_xray, method, ...])	
main()	

class edtools.scattering_factor.**FitResult_4p**(*a0*, *b0*, *a1*, *b1*, *a2*, *b2*, *a3*, *b3*, *c*)

Bases: tuple

Attributes:

a0	Alias for field number 0
a1	Alias for field number 2
a2	Alias for field number 4
a3	Alias for field number 6
b0	Alias for field number 1
b1	Alias for field number 3
b2	Alias for field number 5
b3	Alias for field number 7
c	Alias for field number 8

property a0

Alias for field number 0

property a1

Alias for field number 2

property a2

Alias for field number 4

property a3

Alias for field number 6

property b0

Alias for field number 1

property b1

Alias for field number 3

property b2

Alias for field number 5

property b3

Alias for field number 7

property c

Alias for field number 8

class edtools.scattering_factor.**FitResult_5p**(*a0*, *b0*, *a1*, *b1*, *a2*, *b2*, *a3*, *b3*, *a4*, *b4*, *c*)

Bases: tuple

Attributes:

a0	Alias for field number 0
a1	Alias for field number 2
a2	Alias for field number 4
a3	Alias for field number 6
a4	Alias for field number 8
b0	Alias for field number 1
b1	Alias for field number 3
b2	Alias for field number 5
b3	Alias for field number 7
b4	Alias for field number 9
c	Alias for field number 10

property a0
Alias for field number 0

property a1
Alias for field number 2

property a2
Alias for field number 4

property a3
Alias for field number 6

property a4
Alias for field number 8

property b0
Alias for field number 1

property b1
Alias for field number 3

property b2
Alias for field number 5

property b3
Alias for field number 7

property b4
Alias for field number 9

property c
Alias for field number 10

class edtools.scattering_factor.ScatteringFactorGUI(*parent*)
Bases: Labelframe

A GUI frame for scattering factor

Methods:

__init__(parent)	Construct a Ttk Labelframe with parent master.
clear_plot()	
draw()	
fit_4_param()	
fit_5_param()	
func_4p(param, s)	
func_4p_charge(param, s[, charge])	
func_5p(param, s)	
func_5p_charge(param, s[, charge])	
get_parameters(scat_lib, source, atom, charge)	
init_vars()	
load_lib()	
output()	
plot()	
read()	
select_element(element)	

__init__(*parent*)

Construct a Ttk Labelframe with parent master.

STANDARD OPTIONS

class, cursor, style, takefocus

WIDGET-SPECIFIC OPTIONS

labelanchor, text, underline, padding, labelwidget, width, height

clear_plot()

draw()

fit_4_param()

fit_5_param()

func_4p(*param*, *s*)

func_4p_charge(*param*, *s*, *charge=0*)

func_5p(*param*, *s*)

func_5p_charge(*param*, *s*, *charge=0*)

get_parameters(*scat_lib*, *source*, *atom*, *charge*)

init_vars()

load_lib()

output()

plot()

read()

select_element(*element*)

edtools.scattering_factor.**fit_4_param**(*s*, *target*, *is_xray=False*, *method: str = 'leastsq'*, *verbose: bool = False*, ***param*)

edtools.scattering_factor.**fit_5_param**(*s*, *target*, *is_xray=False*, *method: str = 'leastsq'*, *verbose: bool = False*, ***param*)

edtools.scattering_factor.**main**()

9.1.14 edtools.update_xds

Functions:

main()	
update_xds(fn[, cell, spgr, comment, ...])	

edtools.update_xds.**main**()

edtools.update_xds.**update_xds**(*fn*, *cell=None*, *spgr=None*, *comment=False*, *axis_error=None*, *angle_error=None*, *overload=None*, *lo_res=None*, *hi_res=None*, *cut_frames=None*, *wfac1=None*, *apd=None*, *jobs=None*, *sp=None*, *indnumthre=None*, *d=False*, *dl=None*, *processors=None*, *center=None*, *axis=None*, *cam_len=None*, *mosaicity=None*, *pixel_size=None*, *untrusted=None*, *corr=None*, *refine_idx=None*, *refine_integrate=None*, *refine_corr=None*, *trusted_region=None*, *trusted_pixels=None*)

9.1.15 edtools.utils

Functions:

parse_args_for_fns(args[, name, match])	Parse list of filenames and resolve wildcards name: Name of the file to locate match: Match the file list against the provided glob-style pattern. If the match is False, the path is removed from the list. example: match="SMV_reprocessed".
space_group_lib()	Initialize simple space group library mapping the space group number to a dict with information on the *class* (crystal class), *lattice* (lattice symbol), *laue_symmetry* (number of the lowest symmetry space group for this lattice), *name* (space group name), and *number* (space group number).
volume(cell)	Returns volume for the general case from cell parameters

edtools.utils.**parse_args_for_fns**(*args*, *name='XDS.INP'*, *match=None*)

Parse list of filenames and resolve wildcards name:

Name of the file to locate

match:
Match the file list against the provided glob-style pattern. If the match is False, the path is removed from the list. example:

match="SMV_reprocessed"

edtools.utils.**space_group_lib**()

Initialize simple space group library mapping the space group number to a dict with information on the *class* (crystal class), *lattice* (lattice symbol), *laue_symmetry* (number of the lowest symmetry space group for this lattice), *name* (space group name), and *number* (space group number).

edtools.utils.**volume**(*cell*)

Returns volume for the general case from cell parameters

9.1.16 edtools.widgets

Classes:

Hoverbox(widget[, text])	create a tooltip for a given widget
Spinbox([master])	Ttk Spinbox is an Entry with increment and decrement arrows It is commonly used for number entry or to select from a list of string values.

class edtools.widgets.**Hoverbox**(*widget*, *text='widget info'*)

Bases: object

create a tooltip for a given widget

Methods:

__init__(widget[, text])	
enter([event])	
hidetip()	
leave([event])	
schedule()	
showtip([event])	
unschedule()	

__init__(*widget*, *text='widget info'*)

enter(*event=None*)

hidetip()

leave(*event=None*)

schedule()

showtip(*event=None*)

unschedule()

class edtools.widgets.**Spinbox**(*master=None*, ***kw*)

Bases: Entry

Ttk Spinbox is an Entry with increment and decrement arrows It is commonly used for number entry or to select from a list of string values.

Methods:

__init__([master])	Construct a Ttk Spinbox widget with the parent master.
set(value)	Sets the value of the Spinbox to value.

__init__(*master=None*, ***kw*)

Construct a Ttk Spinbox widget with the parent master.

STANDARD OPTIONS: class, cursor, style, takefocus, validate, validatecommand, xscrollcommand, invalidcommand

WIDGET-SPECIFIC OPTIONS: to, **from_**, increment, values, wrap, format, command

set(*value*)

Sets the value of the Spinbox to value.

9.1.17 edtools.wsl

CHAPTER

TEN

EXAMPLES

10.1 *edtools* Demo

edtools is a python package for automated processing of a large number of 3D electron diffraction (3D ED) datasets. It can be downloaded from https://doi.org/10.5281/zenodo.6952810.

For runing *edtools*, *XDS* package for reduction of 3D ED datasets is required. *XDS* package is available at https://xds.mr.mpg.de/html_doc/downloading.html.

A typical cycle of using *edtools* for processing batch 3D ED datasets goes through the following steps:

- `edtools.autoindex`
- `edtools.extract_xds_info`
- `edtools.find_cell`
- `edtools.update_xds`
- `edtools.make_xscale`
- `edtools.cluster`

Here we demonstrate the processing of batch 3D ED datasets for phase analysis and structure determination using *edtools*. The datasets for the demo can be downloaded from https://zenodo.org/record/6533426#.YnoQ7_hBxaQ.

The datasets were collected on a zeolite mixture sample using serial rotation electron diffraction (SerialRED) data collection technique implemented in the program **Instamatic** (available at https://doi.org/10.5281/zenodo.5175957), which runs on a JEOL JEM-2100-LaB6 at 200 kV equipped with a 512 x 512 Timepix hybrid pixel detector (55 x 55 μm pixel size, QTPX-262k, Amsterdam Scientific Instruments).

The zeolite mixture sample contains phases **IWVRTH**, and ***CTH**. The information of these three phases can be found from the structure database of zeolites (https://europe.iza-structure.org/IZA-SC/ftc_table.php).

This demo takes around 5-10 min to run on a normal desktop computer with all the required packages installed properly beforehand.

10.1.1 Indexing

Automatically index the 3D ED datasets by running *XDS* in all subfolders (SMV) that contains file `XDS.INP`, which is automatically generated during data collection using *Instamatic*.

[1]:
```
!edtools.autoindex
```

```
 !!! ERROR !!! WRONG TYPE OF INPUT FILE SPECIFIED
 !!! ERROR !!! WRONG TYPE OF INPUT FILE SPECIFIED
16 files named XDS.INP (subdir: None) found.

   0: C:\demo\edtools_demo_data\stagepos_0067\crystal_0001\SMV  # Mon Aug  1 21:00:56␣
↪2022
Spgr    5 - Cell      26.93     14.05      5.36     90.00     90.89     90.00 - Vol    ␣
↪2027.80

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
-------------------------------------------------------------------------------
   0   4.35  0.80     583     324    15.0    4.59    13.7    99.0    7.47    6.72
   -   0.85  0.80      54      42    12.5    1.96    26.8    91.9


   1: C:\demo\edtools_demo_data\stagepos_0164\crystal_0000\SMV  # Mon Aug  1 21:00:58␣
↪2022
Spgr    1 - Cell       9.49      9.90     12.47     66.56     89.45     86.35 - Vol    ␣
↪1072.59

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   1   6.39  0.80     229     209     4.8   24.01    22.3    96.3   50.00    4.74
   -   0.91  0.85      31      29     4.5   12.16    21.3     0.0


   3: C:\demo\edtools_demo_data\stagepos_0299\crystal_0001\SMV  # Mon Aug  1 21:01:00␣
↪2022
Spgr    1 - Cell       4.83     14.83     16.03    115.66     89.61     94.16 - Vol    ␣
↪1031.87

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   3   2.05  0.80     400     312     7.5    2.44    20.6    95.2    4.24    6.11
   -   0.84  0.80      27      26     4.7    1.79    11.2     0.0


   4: C:\demo\edtools_demo_data\stagepos_0325\crystal_0000\SMV  # Mon Aug  1 21:01:02␣
↪2022
Spgr    5 - Cell      13.69     25.42     14.90     90.00    115.84     90.00 - Vol    ␣
↪4666.87

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   4  11.09  0.79    3744    2147    42.8    3.44    13.1    99.6   13.90    8.10
   -   0.97  0.90     623     336    47.9    1.32    68.9    84.7


   5: C:\demo\edtools_demo_data\stagepos_0341\crystal_0000\SMV  # Mon Aug  1 21:01:03␣
```

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```
↪2022
Spgr    5 - Cell      25.67     13.50     17.73     90.00    132.44     90.00 - Vol    ␣
↪4534.43

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   5   6.86  0.80    2161    1081    21.8    4.23    10.5    99.9   33.30    8.74
   -   0.97  0.90     342     159    23.3    0.83   130.3    69.6


   6: C:\demo\edtools_demo_data\stagepos_0368\crystal_0001\SMV  # Mon Aug  1 21:01:05␣
↪2022
Spgr    1 - Cell      10.17     10.36     12.16     93.71    113.40     98.01 - Vol    ␣
↪1154.16

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   6  10.17  0.80     611     443     9.4    3.17    14.9    97.5    5.07    4.64
   -   0.85  0.80      56      53     7.0    1.96    73.1     6.4


   7: C:\demo\edtools_demo_data\stagepos_0538\crystal_0000\SMV  # Mon Aug  1 21:01:06␣
↪2022
Spgr    1 - Cell      10.55     10.52     11.81     80.39     66.60     75.74 - Vol    ␣
↪1162.33

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   7   5.10  0.80     443     330     7.0    3.80    10.7    99.4    8.61    5.62
   -   0.85  0.80      38      36     4.8    1.80    76.5     0.0


   8: C:\demo\edtools_demo_data\stagepos_0648\crystal_0001\SMV  # Mon Aug  1 21:01:07␣
↪2022
Spgr    1 - Cell      13.82     14.32     16.18     86.20    111.75    116.39 - Vol    ␣
↪2645.41

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   8   6.37  0.80    1460     989     9.1    2.88    16.3    97.8    5.24    7.62
   -   0.85  0.80     166     125     7.3    1.36    62.8    56.0


   9: C:\demo\edtools_demo_data\stagepos_0849\crystal_0000\SMV  # Mon Aug  1 21:01:08␣
↪2022
Spgr    5 - Cell      15.06     26.22     15.41     90.00    118.30     90.00 - Vol    ␣
↪5357.50

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   9  13.11  0.79    2063    1319    22.1    3.46    10.5    99.6   12.09    7.58
   -   0.89  0.83     326     223    24.5    1.01    53.6    83.4


  10: C:\demo\edtools_demo_data\stagepos_0905\crystal_0000\SMV  # Mon Aug  1 21:01:10␣
↪2022
Spgr    3 - Cell      13.91      5.07     14.97     90.00    117.96     90.00 - Vol    ␣
```

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```
↪932.53

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
  10  12.33  0.80     479     300    13.8    3.68    13.4    99.6   16.07    9.46
   -   1.20  1.07      58      35    14.6    4.72    24.9    88.5


  11: C:\demo\edtools_demo_data\stagepos_0905\crystal_0001\SMV  # Mon Aug  1 21:01:11␣
↪2022
Spgr    1 - Cell      13.71     14.57     15.77     83.07     68.29     62.34 - Vol    ␣
↪2587.36

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
  11  11.49  0.80    1596    1144    10.7    3.30    12.4    98.5    7.24    7.18
   -   0.85  0.80     124     121     7.0    0.94    22.6    83.4


  12: C:\demo\edtools_demo_data\stagepos_0980\crystal_0000\SMV  # Mon Aug  1 21:01:13␣
↪2022
Spgr    1 - Cell      14.56     15.00     15.27     97.22    105.97    120.36 - Vol    ␣
↪2621.77

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
  12   7.54  0.80    1746    1222    11.3    4.00    13.3    98.6    8.77    5.85
   -   0.85  0.80     164     146     8.4    1.48    36.5    86.5


  13: C:\demo\edtools_demo_data\stagepos_1014\crystal_0000\SMV  # Mon Aug  1 21:01:14␣
↪2022
Spgr    1 - Cell       5.30     14.56     15.04    112.06     93.44     86.65 - Vol    ␣
↪1072.87

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
  13   5.01  0.81     447     328     7.5    4.11    10.9    98.5    6.65    6.67
   -   0.85  0.80      51      44     6.3    2.11    18.7    92.7


  15: C:\demo\edtools_demo_data\stagepos_1283\crystal_0001\SMV  # Mon Aug  1 21:01:17␣
↪2022
Spgr    1 - Cell      13.64     15.02     25.09     93.07     91.13    114.33 - Vol    ␣
↪4672.25

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
  15   6.60  0.80    3124    2149    11.3    3.54     8.4    99.5   12.64    6.94
   -   0.85  0.80     346     280     9.2    1.24    56.2    84.9
```

10.1.2 Extract cell

Extract the determined unit cell parameters from the output files (`CORRECT.LP`) of *XDS*

[2]:
```
!edtools.extract_xds_info
```

```
14 files named CORRECT.LP (subdir: None) found.
   1: C:\demo\edtools_demo_data\stagepos_0067\crystal_0001\SMV  # Mon Aug  1 21:00:56␣
↪2022
Spgr    5 - Cell      26.93     14.05      5.36     90.00     90.89     90.00 - Vol   ␣
↪2027.80

   2: C:\demo\edtools_demo_data\stagepos_0164\crystal_0000\SMV  # Mon Aug  1 21:00:58␣
↪2022
Spgr    1 - Cell       9.49      9.90     12.47     66.56     89.45     86.35 - Vol   ␣
↪1072.59

   3: C:\demo\edtools_demo_data\stagepos_0299\crystal_0001\SMV  # Mon Aug  1 21:01:00␣
↪2022
Spgr    1 - Cell       4.83     14.83     16.03    115.66     89.61     94.16 - Vol   ␣
↪1031.87

   4: C:\demo\edtools_demo_data\stagepos_0325\crystal_0000\SMV  # Mon Aug  1 21:01:02␣
↪2022
Spgr    5 - Cell      13.69     25.42     14.90     90.00    115.84     90.00 - Vol   ␣
↪4666.87

   5: C:\demo\edtools_demo_data\stagepos_0341\crystal_0000\SMV  # Mon Aug  1 21:01:03␣
↪2022
Spgr    5 - Cell      25.67     13.50     17.73     90.00    132.44     90.00 - Vol   ␣
↪4534.43

   6: C:\demo\edtools_demo_data\stagepos_0368\crystal_0001\SMV  # Mon Aug  1 21:01:05␣
↪2022
Spgr    1 - Cell      10.17     10.36     12.16     93.71    113.40     98.01 - Vol   ␣
↪1154.16

   7: C:\demo\edtools_demo_data\stagepos_0538\crystal_0000\SMV  # Mon Aug  1 21:01:06␣
↪2022
Spgr    1 - Cell      10.55     10.52     11.81     80.39     66.60     75.74 - Vol   ␣
↪1162.33

   8: C:\demo\edtools_demo_data\stagepos_0648\crystal_0001\SMV  # Mon Aug  1 21:01:07␣
↪2022
Spgr    1 - Cell      13.82     14.32     16.18     86.20    111.75    116.39 - Vol   ␣
↪2645.41

   9: C:\demo\edtools_demo_data\stagepos_0849\crystal_0000\SMV  # Mon Aug  1 21:01:08␣
↪2022
Spgr    5 - Cell      15.06     26.22     15.41     90.00    118.30     90.00 - Vol   ␣
↪5357.50

  10: C:\demo\edtools_demo_data\stagepos_0905\crystal_0000\SMV  # Mon Aug  1 21:01:10␣
↪2022
```

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```
Spgr    3 - Cell      13.91      5.07     14.97     90.00    117.96     90.00 - Vol    ␣
↪932.53

  11: C:\demo\edtools_demo_data\stagepos_0905\crystal_0001\SMV  # Mon Aug  1 21:01:11␣
↪2022
Spgr    1 - Cell      13.71     14.57     15.77     83.07     68.29     62.34 - Vol    ␣
↪2587.36

  12: C:\demo\edtools_demo_data\stagepos_0980\crystal_0000\SMV  # Mon Aug  1 21:01:13␣
↪2022
Spgr    1 - Cell      14.56     15.00     15.27     97.22    105.97    120.36 - Vol    ␣
↪2621.77

  13: C:\demo\edtools_demo_data\stagepos_1014\crystal_0000\SMV  # Mon Aug  1 21:01:14␣
↪2022
Spgr    1 - Cell       5.30     14.56     15.04    112.06     93.44     86.65 - Vol    ␣
↪1072.87

  14: C:\demo\edtools_demo_data\stagepos_1283\crystal_0001\SMV  # Mon Aug  1 21:01:17␣
↪2022
Spgr    1 - Cell      13.64     15.02     25.09     93.07     91.13    114.33 - Vol    ␣
↪4672.25

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
-------------------------------------------------------------------------------

   1   4.35  0.80     583     324    15.0    4.59    13.7    99.0    7.47    6.72  # C:\
↪demo\edtools_demo_data\stagepos_0067\crystal_0001\SMV\CORRECT.LP
   -   0.85  0.80      54      42    12.5    1.96    26.8    91.9

   2   6.39  0.80     229     209     4.8   24.01    22.3    96.3   50.00    4.74  # C:\
↪demo\edtools_demo_data\stagepos_0164\crystal_0000\SMV\CORRECT.LP
   -   0.91  0.85      31      29     4.5   12.16    21.3     0.0

   3   2.05  0.80     400     312     7.5    2.44    20.6    95.2    4.24    6.11  # C:\
↪demo\edtools_demo_data\stagepos_0299\crystal_0001\SMV\CORRECT.LP
   -   0.84  0.80      27      26     4.7    1.79    11.2     0.0

   4  11.09  0.79    3744    2147    42.8    3.44    13.1    99.6   13.90    8.10  # C:\
↪demo\edtools_demo_data\stagepos_0325\crystal_0000\SMV\CORRECT.LP
   -   0.97  0.90     623     336    47.9    1.32    68.9    84.7

   5   6.86  0.80    2161    1081    21.8    4.23    10.5    99.9   33.30    8.74  # C:\
↪demo\edtools_demo_data\stagepos_0341\crystal_0000\SMV\CORRECT.LP
   -   0.97  0.90     342     159    23.3    0.83   130.3    69.6

   6  10.17  0.80     611     443     9.4    3.17    14.9    97.5    5.07    4.64  # C:\
↪demo\edtools_demo_data\stagepos_0368\crystal_0001\SMV\CORRECT.LP
   -   0.85  0.80      56      53     7.0    1.96    73.1     6.4

   7   5.10  0.80     443     330     7.0    3.80    10.7    99.4    8.61    5.62  # C:\
↪demo\edtools_demo_data\stagepos_0538\crystal_0000\SMV\CORRECT.LP
```

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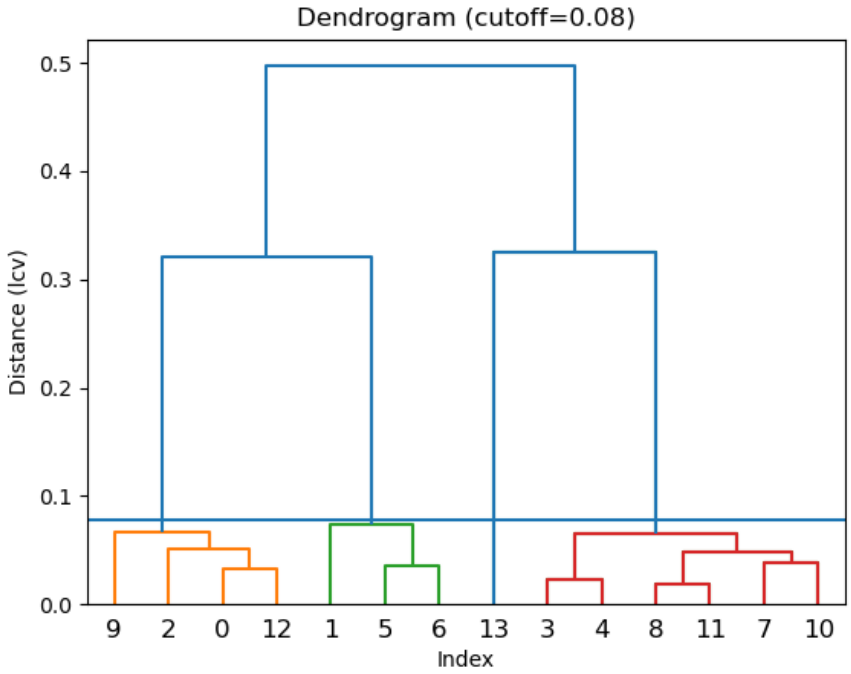
```
   -    0.85  0.80      38      36     4.8    1.80    76.5     0.0

   8    6.37  0.80    1460     989     9.1    2.88    16.3    97.8    5.24    7.62  # C:\
↪demo\edtools_demo_data\stagepos_0648\crystal_0001\SMV\CORRECT.LP
   -    0.85  0.80     166     125     7.3    1.36    62.8    56.0

   9   13.11  0.79    2063    1319    22.1    3.46    10.5    99.6   12.09    7.58  # C:\
↪demo\edtools_demo_data\stagepos_0849\crystal_0000\SMV\CORRECT.LP
   -    0.89  0.83     326     223    24.5    1.01    53.6    83.4

  10   12.33  0.80     479     300    13.8    3.68    13.4    99.6   16.07    9.46  # C:\
↪demo\edtools_demo_data\stagepos_0905\crystal_0000\SMV\CORRECT.LP
   -    1.20  1.07      58      35    14.6    4.72    24.9    88.5

  11   11.49  0.80    1596    1144    10.7    3.30    12.4    98.5    7.24    7.18  # C:\
↪demo\edtools_demo_data\stagepos_0905\crystal_0001\SMV\CORRECT.LP
   -    0.85  0.80     124     121     7.0    0.94    22.6    83.4

  12    7.54  0.80    1746    1222    11.3    4.00    13.3    98.6    8.77    5.85  # C:\
↪demo\edtools_demo_data\stagepos_0980\crystal_0000\SMV\CORRECT.LP
   -    0.85  0.80     164     146     8.4    1.48    36.5    86.5

  13    5.01  0.81     447     328     7.5    4.11    10.9    98.5    6.65    6.67  # C:\
↪demo\edtools_demo_data\stagepos_1014\crystal_0000\SMV\CORRECT.LP
   -    0.85  0.80      51      44     6.3    2.11    18.7    92.7

  14    6.60  0.80    3124    2149    11.3    3.54     8.4    99.5   12.64    6.94  # C:\
↪demo\edtools_demo_data\stagepos_1283\crystal_0001\SMV\CORRECT.LP
   -    0.85  0.80     346     280     9.2    1.24    56.2    84.9

Wrote 14 cells to file cells.xlsx
Wrote 14 cells to file cells.yaml
Wrote 8 entries to file filelist.txt (completeness > 10.0%, CC(1/2) > 90.0%)

Most likely lattice types:
  1 Lattice type `aP` (spgr:   1) was found   9 times (score:   10056)
  2 Lattice type `mC` (spgr:   5) was found   4 times (score:    8551)
  3 Lattice type `mP` (spgr:   3) was found   1 times (score:     479)

 ** the score corresponds to the total number of indexed reflections.
```

10.1.3 Unit-cell-based clustering for phase analysis

[ ]:
```
!edtools.find_cell cells.yaml -s --cluster --metric lcv
```

[3]:
```
from IPython.display import Image
Image('find_cell_step3.png', embed=True)
```



nbsphinx-code-borderwidth

Console Output

```
Linkage method = average
Cutoff distance = 0.078
Distance metric = lcv

----------------------------------------

Cluster #1 (4 items)
    1 [   5.47   14.07   15.30   63.22   87.59   88.58]  Vol.: 1050.9
    3 [   5.33   14.99   16.06   64.44   89.16   82.51]  Vol.: 1144.9
   10 [   5.05   14.37   14.53   62.13   88.52   89.11]  Vol.:  932.0
   13 [   5.30   14.89   15.18   66.79   86.51   86.59]  Vol.: 1098.1
 ---
Mean: [   5.29   14.58   15.27   64.15   87.95   86.70]  Vol.: 1056.5
 Min: [   5.05   14.07   14.53   62.13   86.51   82.51]  Vol.:  932.0
 Max: [   5.47   14.99   16.06   66.79   89.16   89.11]  Vol.: 1144.9

Cluster #2 (3 items)
    2 [   9.52    9.98   12.85   65.60   87.80   85.43]  Vol.: 1107.8
    6 [  10.21   10.36   12.08   85.86   67.02   81.83]  Vol.: 1165.3
    7 [  10.55   10.75   11.75   80.34   66.42   75.73]  Vol.: 1179.4
 ---
Mean: [  10.09   10.36   12.23   77.27   73.75   81.00]  Vol.: 1150.9
 Min: [   9.52    9.98   11.75   65.60   66.42   75.73]  Vol.: 1107.8
 Max: [  10.55   10.75   12.85   85.86   87.80   85.43]  Vol.: 1179.4

Cluster #3 (6 items)
    4 [  14.04   14.39   14.72   76.68   62.79   61.86]  Vol.: 2331.3
```

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```
    5 [  13.50   14.38   14.63   75.73   64.60   63.07]  Vol.: 2283.0
    8 [  13.89   14.29   17.00   72.43   63.61   63.57]  Vol.: 2684.8
    9 [  14.81   15.07   15.52   62.45   74.78   62.16]  Vol.: 2711.1
   11 [  13.73   14.56   16.03   84.26   68.05   62.57]  Vol.: 2629.5
   12 [  14.43   14.90   15.40   81.24   74.01   61.15]  Vol.: 2787.8
 ---
Mean: [  14.07   14.60   15.55   75.46   67.97   62.40]  Vol.: 2571.3
 Min: [  13.50   14.29   14.63   62.45   62.79   61.15]  Vol.: 2283.0
 Max: [  14.81   15.07   17.00   84.26   74.78   63.57]  Vol.: 2787.8

Wrote cluster 1 to file `cells_cluster_1_4-items.yaml`
Wrote cluster 2 to file `cells_cluster_2_3-items.yaml`
Wrote cluster 3 to file `cells_cluster_3_6-items.yaml`
```

The three resulted clusters 1, 2, 3 correspond to phases *__CTH__, __RTH__, and __IWV__, respectively.

With the averaged primitive unit cell parameters of each cluster, one can use the online tool http://cci.lbl.gov/cctbx/lattice_symmetry.html to find unit cell with higher symmetry with a pre-set tolerance.

We take cluster 3 (phase __IWV__) as an example. The averaged unit cell parameters are: 14.07, 14.6, 15.55, 75.46, 67.97, 62.40

The unit cell parameters with a higher symmetry (space group: *Fmmm* (69)) are: 14.07, 25.8828, 28.9294, 90, 90, 90

The same operation can be done for all the other clusters.

10.1.4 Update the *XDS.INP* files

This step used `edtools.update_xds` to update the XDS input files with the determined unit cell parameters and space group.

[4]:
```
!edtools.update_xds -c 14.07 25.8828 28.9294 90 90 90 -s 69
```

```
16 files named XDS.INP (subdir: None) found.
 C:\demo\edtools_demo_data\stagepos_0067\crystal_0001\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0164\crystal_0000\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0290\crystal_0002\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0299\crystal_0001\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0325\crystal_0000\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0341\crystal_0000\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0368\crystal_0001\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0538\crystal_0000\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0648\crystal_0001\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0849\crystal_0000\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0905\crystal_0000\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0905\crystal_0001\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_0980\crystal_0000\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_1014\crystal_0000\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_1261\crystal_0001\SMV\XDS.INP
 C:\demo\edtools_demo_data\stagepos_1283\crystal_0001\SMV\XDS.INP
Updated 16 files
```

10.1.5 Refine phases

Rerun **autoindex**, **extract_xds_info** and **find_cell** for the desired phases to be successfully indexed by *XDS*. All the other phases are hopefully excluded in that a phase with different enough unit cell will not be indexed successfully. There are however cases when different phases have similar unit cells, which cannot be told apart during this step.

[5]:
```
!edtools.autoindex
```

```
 !!! ERROR !!! WRONG TYPE OF INPUT FILE SPECIFIED
 !!! ERROR !!! WRONG TYPE OF INPUT FILE SPECIFIED
16 files named XDS.INP (subdir: None) found.

   4: C:\demo\edtools_demo_data\stagepos_0325\crystal_0000\SMV  # Mon Aug  1 21:03:22␣
↪2022
Spgr   69 - Cell      13.88     25.44     27.26     90.00     90.00     90.00 - Vol   ␣
↪9625.70

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   4   9.30  0.80    3938    1852    69.0    3.24    20.2    99.4   11.45    8.21
   -   0.91  0.85     614     290    74.4    0.86   109.5    81.7


   5: C:\demo\edtools_demo_data\stagepos_0341\crystal_0000\SMV  # Mon Aug  1 21:03:24␣
↪2022
Spgr   69 - Cell      13.52     24.94     27.07     90.00     90.00     90.00 - Vol   ␣
↪9127.70

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   5  10.88  0.80    2203    1029    40.4    3.84    11.7    99.9   27.38    9.78
   -   1.07  0.98     299     135    41.8    1.04   107.2    76.5


   8: C:\demo\edtools_demo_data\stagepos_0648\crystal_0001\SMV  # Mon Aug  1 21:03:28␣
↪2022
Spgr   69 - Cell      14.01     25.97     29.04     90.00     90.00     90.00 - Vol   ␣
↪10565.90

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   8   7.14  0.80    1466     781    26.2    2.61    18.2    97.2    4.73    7.15
   -   0.84  0.80     142      92    19.9    0.98    62.3    52.7


   9: C:\demo\edtools_demo_data\stagepos_0849\crystal_0000\SMV  # Mon Aug  1 21:03:30␣
↪2022
Spgr   69 - Cell      15.10     26.02     26.72     90.00     90.00     90.00 - Vol   ␣
↪10498.34

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
   9   7.24  0.80    1994    1126    38.5    3.27    11.9    99.5   12.91    8.08
   -   0.98  0.90     322     166    41.2    1.27    70.2    89.0

  10: C:\demo\edtools_demo_data\stagepos_0905\crystal_0000\SMV -> Error in IDXREF:␣
↪RETURN CODE IS IER=           0
```

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```
  11: C:\demo\edtools_demo_data\stagepos_0905\crystal_0001\SMV  # Mon Aug  1 21:03:32␣
↪2022
Spgr   69 - Cell      13.83     25.80     28.73     90.00     90.00     90.00 - Vol  ␣
↪10251.27

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
  11   7.08  0.80    1591     808    28.2    2.88    17.1    98.1    6.24    7.63
   -   0.90  0.85     254     128    30.4    1.17    42.6    95.4


  12: C:\demo\edtools_demo_data\stagepos_0980\crystal_0000\SMV  # Mon Aug  1 21:03:34␣
↪2022
Spgr   69 - Cell      14.39     25.16     28.10     90.00     90.00     90.00 - Vol  ␣
↪10173.67

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
  12   5.12  0.80    1669     851    30.2    3.75    16.8    98.0    6.26    5.76
   -   0.85  0.80     153     109    25.3    1.34    46.1    68.5


  15: C:\demo\edtools_demo_data\stagepos_1283\crystal_0001\SMV  # Mon Aug  1 21:03:39␣
↪2022
Spgr   69 - Cell      13.54     25.23     27.30     90.00     90.00     90.00 - Vol  ␣
↪9326.07

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
  15   5.97  0.80    1620     563    21.7    6.15     8.4    99.8   11.79    7.17
   -   0.85  0.80     187      78    19.1    2.24    45.1    97.9
```

[6]:
```
!edtools.extract_xds_info
```

```
7 files named CORRECT.LP (subdir: None) found.
   1: C:\demo\edtools_demo_data\stagepos_0325\crystal_0000\SMV  # Mon Aug  1 21:03:22␣
↪2022
Spgr   69 - Cell      13.88     25.44     27.26     90.00     90.00     90.00 - Vol  ␣
↪9625.70

   2: C:\demo\edtools_demo_data\stagepos_0341\crystal_0000\SMV  # Mon Aug  1 21:03:24␣
↪2022
Spgr   69 - Cell      13.52     24.94     27.07     90.00     90.00     90.00 - Vol  ␣
↪9127.70

   3: C:\demo\edtools_demo_data\stagepos_0648\crystal_0001\SMV  # Mon Aug  1 21:03:28␣
↪2022
Spgr   69 - Cell      14.01     25.97     29.04     90.00     90.00     90.00 - Vol  ␣
↪10565.90

   4: C:\demo\edtools_demo_data\stagepos_0849\crystal_0000\SMV  # Mon Aug  1 21:03:30␣
↪2022
Spgr   69 - Cell      15.10     26.02     26.72     90.00     90.00     90.00 - Vol  ␣
↪10498.34
```

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```
   5: C:\demo\edtools_demo_data\stagepos_0905\crystal_0001\SMV  # Mon Aug  1 21:03:32␣
↪2022
Spgr   69 - Cell      13.83     25.80     28.73     90.00     90.00     90.00 - Vol  ␣
↪10251.27

   6: C:\demo\edtools_demo_data\stagepos_0980\crystal_0000\SMV  # Mon Aug  1 21:03:34␣
↪2022
Spgr   69 - Cell      14.39     25.16     28.10     90.00     90.00     90.00 - Vol  ␣
↪10173.67

   7: C:\demo\edtools_demo_data\stagepos_1283\crystal_0001\SMV  # Mon Aug  1 21:03:39␣
↪2022
Spgr   69 - Cell      13.54     25.23     27.30     90.00     90.00     90.00 - Vol   ␣
↪9326.07

   #   dmax  dmin    ntot   nuniq   compl   i/sig   rmeas CC(1/2)     ISa   B(ov)
-------------------------------------------------------------------------------

   1   9.30  0.80    3938    1852    69.0    3.24    20.2    99.4   11.45    8.21  # C:\
↪demo\edtools_demo_data\stagepos_0325\crystal_0000\SMV\CORRECT.LP
   -   0.91  0.85     614     290    74.4    0.86   109.5    81.7

   2  10.88  0.80    2203    1029    40.4    3.84    11.7    99.9   27.38    9.78  # C:\
↪demo\edtools_demo_data\stagepos_0341\crystal_0000\SMV\CORRECT.LP
   -   1.07  0.98     299     135    41.8    1.04   107.2    76.5

   3   7.14  0.80    1466     781    26.2    2.61    18.2    97.2    4.73    7.15  # C:\
↪demo\edtools_demo_data\stagepos_0648\crystal_0001\SMV\CORRECT.LP
   -   0.84  0.80     142      92    19.9    0.98    62.3    52.7

   4   7.24  0.80    1994    1126    38.5    3.27    11.9    99.5   12.91    8.08  # C:\
↪demo\edtools_demo_data\stagepos_0849\crystal_0000\SMV\CORRECT.LP
   -   0.98  0.90     322     166    41.2    1.27    70.2    89.0

   5   7.08  0.80    1591     808    28.2    2.88    17.1    98.1    6.24    7.63  # C:\
↪demo\edtools_demo_data\stagepos_0905\crystal_0001\SMV\CORRECT.LP
   -   0.90  0.85     254     128    30.4    1.17    42.6    95.4

   6   5.12  0.80    1669     851    30.2    3.75    16.8    98.0    6.26    5.76  # C:\
↪demo\edtools_demo_data\stagepos_0980\crystal_0000\SMV\CORRECT.LP
   -   0.85  0.80     153     109    25.3    1.34    46.1    68.5

   7   5.97  0.80    1620     563    21.7    6.15     8.4    99.8   11.79    7.17  # C:\
↪demo\edtools_demo_data\stagepos_1283\crystal_0001\SMV\CORRECT.LP
   -   0.85  0.80     187      78    19.1    2.24    45.1    97.9

Wrote 7 cells to file cells.xlsx
Wrote 7 cells to file cells.yaml
Wrote 7 entries to file filelist.txt (completeness > 10.0%, CC(1/2) > 90.0%)

Most likely lattice types:
```

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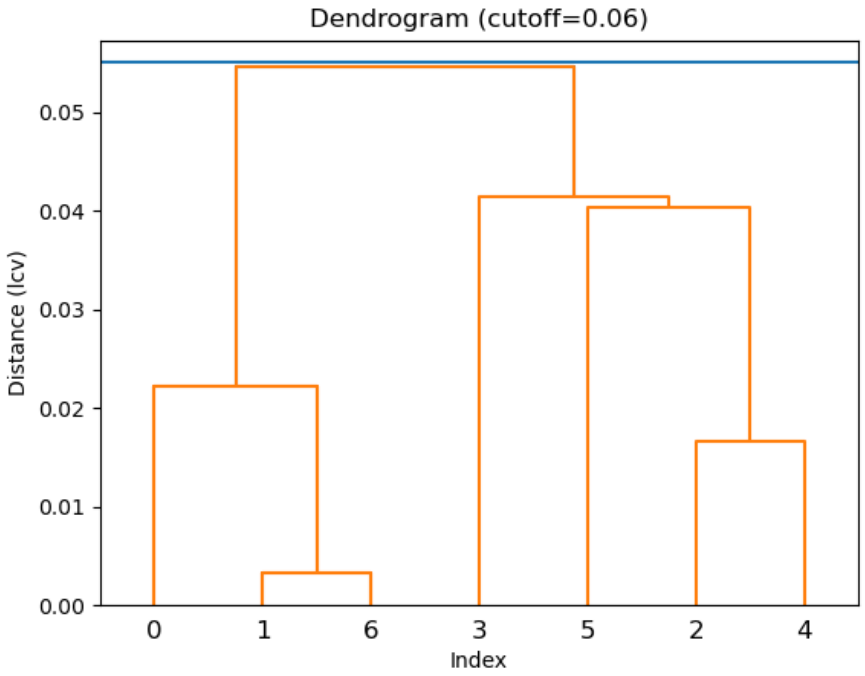
```
  1 Lattice type `oF` (spgr:  22) was found   7 times (score:   14481)

 ** the score corresponds to the total number of indexed reflections.
```

[ ]:
```
!edtools.find_cell cells.yaml --cluster --metric lcv
```

[7]:
```
Image('find_cell_step5.png', embed=True)
```



nbsphinx-code-borderwidth

Console Output

```
Linkage method = average
Cutoff distance = 0.0551
Distance metric = lcv

----------------------------------------

Cluster #1 (7 items)
    1 [  13.97   25.49   27.12   90.00   90.00   90.00]  Vol.: 9657.9
    2 [  13.53   25.01   27.18   90.00   90.00   90.00]  Vol.: 9195.6
    3 [  14.03   26.02   29.55   90.00   90.00   90.00]  Vol.: 10790.3
    4 [  14.94   26.14   26.94   90.00   90.00   90.00]  Vol.: 10522.3
    5 [  13.85   25.79   29.03   90.00   90.00   90.00]  Vol.: 10364.0
    6 [  14.52   24.95   28.11   90.00   90.00   90.00]  Vol.: 10184.6
    7 [  13.53   25.13   27.15   90.00   90.00   90.00]  Vol.: 9233.7
 ---
Mean: [  14.05   25.50   27.87   90.00   90.00   90.00]  Vol.: 9992.6
 Min: [  13.53   24.95   26.94   90.00   90.00   90.00]  Vol.: 9195.6
 Max: [  14.94   26.14   29.55   90.00   90.00   90.00]  Vol.: 10790.3
```

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```
Wrote cluster 1 to file `cells_cluster_1_7-items.yaml`
```

10.1.6 Generate the input file for *XSCALE*

This command generates the desired unit cell cluster for *XSCALE*.

[8]:
```
!edtools.make_xscale cells_cluster_1_7-items.yaml -c 14.05 25.50 27.87 90.00 90.00 90.00␣
↪-s 69
```

```
Loaded 7 cells
Lowest possible symmetry for 69 (oF): 22

Using:
  SPACE_GROUP_NUMBER= 69
  UNIT_CELL_CONSTANTS= 14.050 25.500 27.870 90.000 90.000 90.000

Wrote file XSCALE.INP
Wrote file XDSCONV.INP
```

10.1.7 Run *XSCALE*

XSCALE calculates the correlation coefficients between different datasets.

[9]:
```
!wsl xscale
```

```
 ***** XSCALE ***** (VERSION Jan 10, 2022  BUILT=20220220)   1-Aug-2022
 Author: Wolfgang Kabsch
 Copy licensed until 31-Mar-2023 to
  academic users for non-commercial applications
 No redistribution.


 ******************************************************************************
                               CONTROL CARDS
 ******************************************************************************

 SNRC= 2
 SAVE_CORRECTION_IMAGES= FALSE
 SPACE_GROUP_NUMBER= 69
 UNIT_CELL_CONSTANTS= 14.050 25.500 27.870 90.000 90.000 90.000

 OUTPUT_FILE= MERGED.HKL

     INPUT_FILE= edtools_demo_data/stagepos_0325/crystal_0000/SMV/XDS_ASCII.HKL
     INCLUDE_RESOLUTION_RANGE= 20 0.8

     INPUT_FILE= edtools_demo_data/stagepos_0341/crystal_0000/SMV/XDS_ASCII.HKL
     INCLUDE_RESOLUTION_RANGE= 20 0.8

     INPUT_FILE= edtools_demo_data/stagepos_0648/crystal_0001/SMV/XDS_ASCII.HKL
```

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```
    INCLUDE_RESOLUTION_RANGE= 20 0.8

    INPUT_FILE= edtools_demo_data/stagepos_0849/crystal_0000/SMV/XDS_ASCII.HKL
    INCLUDE_RESOLUTION_RANGE= 20 0.8

    INPUT_FILE= edtools_demo_data/stagepos_0905/crystal_0001/SMV/XDS_ASCII.HKL
    INCLUDE_RESOLUTION_RANGE= 20 0.8

    INPUT_FILE= edtools_demo_data/stagepos_0980/crystal_0000/SMV/XDS_ASCII.HKL
    INCLUDE_RESOLUTION_RANGE= 20 0.8

    INPUT_FILE= edtools_demo_data/stagepos_1283/crystal_0001/SMV/XDS_ASCII.HKL
    INCLUDE_RESOLUTION_RANGE= 20 0.8


 THE DATA COLLECTION STATISTICS REPORTED BELOW ASSUMES:
 SPACE_GROUP_NUMBER=   69
 UNIT_CELL_CONSTANTS=    14.05    25.50    27.87  90.000  90.000  90.000



 ALL DATA SETS WILL BE SCALED TO edtools_demo_data/stagepos_0325/crystal_0000/SMV/XDS_
↪ASCII.HKL


 ******************************************************************************
                    READING INPUT REFLECTION DATA FILES
 ******************************************************************************

 DATA    MEAN       REFLECTIONS        INPUT FILE NAME
 SET# INTENSITY  ACCEPTED REJECTED
   1  0.3010E+02     3938      0  edtools_demo_data/stagepos_0325/crystal_0000/SMV/XDS_
↪ASCII.HKL
   2  0.1368E+02     2205      0  edtools_demo_data/stagepos_0341/crystal_0000/SMV/XDS_
↪ASCII.HKL
   3  0.9168E+02     1453      0  edtools_demo_data/stagepos_0648/crystal_0001/SMV/XDS_
↪ASCII.HKL
   4  0.4279E+02     1931      0  edtools_demo_data/stagepos_0849/crystal_0000/SMV/XDS_
↪ASCII.HKL
   5  0.8542E+02     1590      0  edtools_demo_data/stagepos_0905/crystal_0001/SMV/XDS_
↪ASCII.HKL
   6  0.1676E+03     1662      0  edtools_demo_data/stagepos_0980/crystal_0000/SMV/XDS_
↪ASCII.HKL
   7  0.1915E+03     1620      0  edtools_demo_data/stagepos_1283/crystal_0001/SMV/XDS_
↪ASCII.HKL


 ******************************************************************************
                OVERALL SCALING AND CRYSTAL DISORDER CORRECTION
 ******************************************************************************

      CORRELATIONS BETWEEN INPUT DATA SETS AFTER CORRECTIONS
```

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```
DATA SETS  NUMBER OF COMMON  CORRELATION   RATIO OF COMMON   B-FACTOR
 #i   #j     REFLECTIONS     BETWEEN i,j  INTENSITIES (i/j)  BETWEEN i,j

   1    2         119           0.936           3.1896         0.1394
   1    3          87           0.980           0.5337        -0.4854
   2    3         164           0.945           0.1982        -0.5975
   1    4         216           0.925           1.0428        -0.6421
   2    4         116           0.972           0.3076        -0.4582
   3    4         131           0.894           1.6716         0.0043
   1    5          80           0.959           0.3779         0.1598
   2    5         147           0.970           0.1872        -0.3822
   3    5         218           0.988           0.9850         0.0336
   4    5          96           0.928           0.6114         0.1442
   1    6         206           0.955           0.1970        -0.4620
   2    6          81           0.949           0.0917        -0.7741
   3    6          91           0.934           0.6363        -0.3722
   4    6         106           0.927           0.2401        -0.0297
   5    6          81           0.866           0.5334        -0.1957
   1    7          35           0.965           0.4893        -1.1586
   2    7         131           0.981           0.1113        -1.0633
   3    7         158           0.984           0.5449        -0.3181
   4    7          45           0.833           0.4069        -0.1510
   5    7         196           0.987           0.5649        -0.4493
   6    7          67           0.846           1.6099        -0.5928


K*EXP(B*SS) = Factor applied to intensities
   SS       = (2sin(theta)/lambda)^2

     K         B           DATA SET NAME
 1.000E+00   0.000    edtools_demo_data/stagepos_0325/crystal_0000/SMV/XDS_ASCII.HKL
 2.961E+00   0.170    edtools_demo_data/stagepos_0341/crystal_0000/SMV/XDS_ASCII.HKL
 5.374E-01  -0.365    edtools_demo_data/stagepos_0648/crystal_0001/SMV/XDS_ASCII.HKL
 9.426E-01  -0.465    edtools_demo_data/stagepos_0849/crystal_0000/SMV/XDS_ASCII.HKL
 5.063E-01  -0.243    edtools_demo_data/stagepos_0905/crystal_0001/SMV/XDS_ASCII.HKL
 2.304E-01  -0.530    edtools_demo_data/stagepos_0980/crystal_0000/SMV/XDS_ASCII.HKL
 3.491E-01  -0.812    edtools_demo_data/stagepos_1283/crystal_0001/SMV/XDS_ASCII.HKL

*****************************************************************************
   CORRECTION PARAMETERS FOR THE STANDARD ERROR OF REFLECTION INTENSITIES
*****************************************************************************

The variance v0(I) of the intensity I obtained from counting statistics is
replaced by v(I)=a*(v0(I)+b*I^2). The model parameters a, b are chosen to
minimize the discrepancies between v(I) and the variance estimated from
sample statistics of symmetry related reflections. This model implicates
an asymptotic limit ISa=1/SQRT(a*b) for the highest I/Sigma(I) that the
experimental setup can produce (Diederichs (2010) Acta Cryst D66, 733-740).
Often the value of ISa is reduced from the initial value ISa0 due to systematic
errors showing up by comparison with other data sets in the scaling procedure.
(ISa=ISa0=-1 if v0 is unknown for a data set.)
```

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```
    a        b          ISa    ISa0   INPUT DATA SET
 3.014E+00  1.258E-02    5.14   11.45 edtools_demo_data/stagepos_0325/crystal_0000/SMV/
↪XDS_ASCII.HKL
 2.201E+00  3.743E-03   11.02   27.38 edtools_demo_data/stagepos_0341/crystal_0000/SMV/
↪XDS_ASCII.HKL
 8.809E+00  2.191E-02    2.28    4.73 edtools_demo_data/stagepos_0648/crystal_0001/SMV/
↪XDS_ASCII.HKL
 6.242E+00  1.032E-02    3.94   12.91 edtools_demo_data/stagepos_0849/crystal_0000/SMV/
↪XDS_ASCII.HKL
 7.668E+00  1.817E-02    2.68    6.25 edtools_demo_data/stagepos_0905/crystal_0001/SMV/
↪XDS_ASCII.HKL
 1.379E+01  1.128E-02    2.53    6.26 edtools_demo_data/stagepos_0980/crystal_0000/SMV/
↪XDS_ASCII.HKL
 7.838E-01  1.921E-01    2.58   11.79 edtools_demo_data/stagepos_1283/crystal_0001/SMV/
↪XDS_ASCII.HKL


FACTOR TO PLACE ALL DATA SETS TO AN APPROXIMATE ABSOLUTE SCALE 0.143057E+03
(ASSUMING A PROTEIN WITH 50% SOLVENT)



*****************************************************************************
 STATISTICS OF SCALED OUTPUT DATA SET : MERGED.HKL
 FILE TYPE:         XDS_ASCII      MERGE=FALSE          FRIEDEL'S_LAW=TRUE

       13 OUT OF     14399 REFLECTIONS REJECTED
    14386 REFLECTIONS ON OUTPUT FILE

*****************************************************************************
DEFINITIONS:
R-FACTOR
observed = (SUM(ABS(I(h,i)-I(h))))/(SUM(I(h,i)))
expected = expected R-FACTOR derived from Sigma(I)

COMPARED = number of reflections used for calculating R-FACTOR
I/SIGMA  = mean of intensity/Sigma(I) of unique reflections
           (after merging symmetry-related observations)
Sigma(I) = standard deviation of reflection intensity I
           estimated from sample statistics

R-meas   = redundancy independent R-factor (intensities)
           Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

CC(1/2)  = percentage of correlation between intensities from
           random half-datasets. Correlation significant at
           the 0.1% level is marked by an asterisk.
           Karplus & Diederichs (2012), Science 336, 1030-33
Anomal   = percentage of correlation between random half-sets
 Corr      of anomalous intensity differences. Correlation
           significant at the 0.1% level is marked.
```

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```
 SigAno   = mean anomalous difference in units of its estimated
            standard deviation (|F(+)-F(-)|/Sigma). F(+), F(-)
            are structure factor estimates obtained from the
            merged intensity observations in each parity class.
  Nano    = Number of unique reflections used to calculate
            Anomal_Corr & SigAno. At least two observations
            for each (+ and -) parity are required.


 cpu time used by XSCALE        0.2 sec
 elapsed wall-clock time        0.2 sec
```

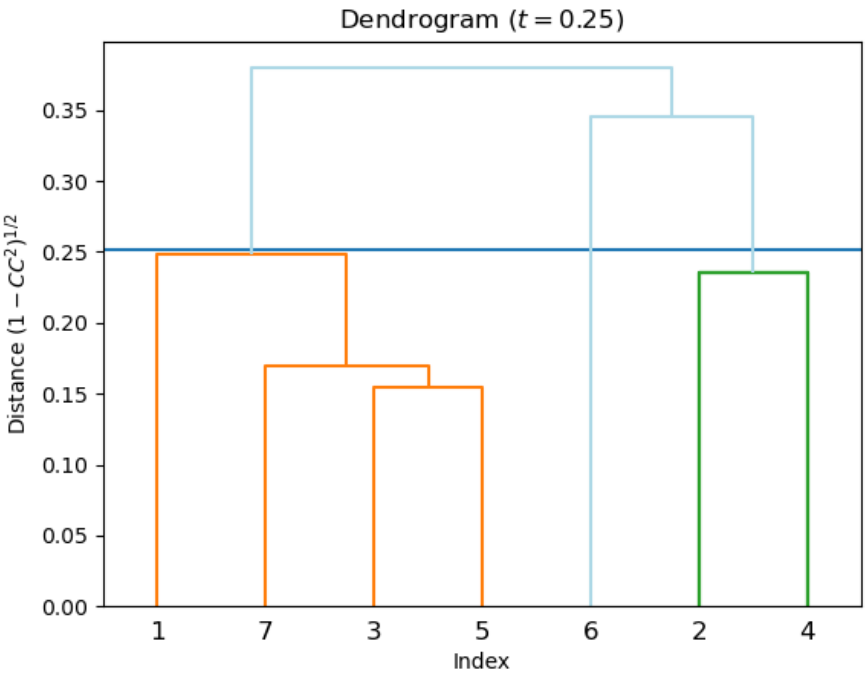
10.1.8 Intensity-based clustering

Run intensity-based clustering to further filter out datasets with low correlation (to remove poor quality datasets), or from a different phase that with similar enough unit cell. Cut-off on the dendrogram is selected manually. A number below 0.4 can be a good starting choice.

In the end, integration results from datasets corresponding to different clusters are automatically copied to different folders after running clustering. The merged intensities in file `shelx.hkl` can be used for structure determination.

[ ]:
```
!edtools.cluster
```

[10]:
```
Image('intensity_cluster.png', embed=True)
```



nbsphinx-code-border[10]

Console Output

```
Running XSCALE on cluster 1
Running XSCALE on cluster 2

Clustering results

Cutoff distance: 0.252
Equivalent CC(I): 0.968
Method: average

  #  N_clust   CC(1/2)    N_obs   N_uniq   N_poss    Compl.   N_comp    R_meas    d_min ␣
↪i/sigma  | Lauegr.  prob. conf.  idx
  2**      2     99.8*     4111     1546     2789     55.4      3723    0.143*     0.80 ␣
↪   3.27
  1***     4     97.3*     8599     2496     2782     89.7*     8220    0.270*     0.80 ␣
↪   2.85
(Sorted by 'Completeness')

Cluster 1: [1, 3, 5, 7]
Cluster 2: [2, 4]
```

10.2 Instruction for using on your own data

- Install **edtools** and all software dependencies on your system
- Put all your 3D ED datasets in one folder. All the 3D ED datasets are expected to be in some *XDS* readable image format, e.g. SMV. A correctly configured *XDS.INP* file is also expected for each dataset.
- Open Windows command prompt from the root directory which contains all the datasets
- Follow the demo

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