Running XDS automatically

USAGE: XDS.py [OPTION]... IMAGE_FILES
FILES is for one or multiple diffraction image files.
OPTIONS:

-h, --help
   Print this help message.

-1, -2, -3, -4, -5
   Jump directly to a particular step (to avoid rerun initial steps):
   -1: XYCOOR + INIT   (Image background analysis)
   -2: COLSPOT   (Collecting spots for indexing)
   -3: IDXREF   (Auto-indexing)
   -4: DEFPIX + INTEGRATE   (Integration)
   -5: CORRECT   (Scaling)

-a, --anomal
   Distinguishes Friedel paires for scaling, strategy and completeness
   statistics. Default is no anoulous contribution.

-r, --high-resolution
   Set a high resolution cutoff. Default is 0 (no cutoff).

-R, --low-resolution
   Set a low resolution cutoff. Default is 9999.

-c, --cell
   Set the expected cell.
   For example: -c "79 79 38 90 90 90"

-s, --spg
   Set the expected space group using either the space group number
   or simple string.
   For example: -s 18 or -s P21212

-i, --xds-input
   Give direct XDS Keyword input.
   For example: -i "DETECTOR_DISTANCE= 167.0 JOB= IDXREF AIR= 0.002"

-b, --beam-center-optimize
   Starting from the initial given values, search and optimize the beam
   center coordinates (given by -x, -y or extracted form the header).

-S, --strategy
   Force to go for calculating strategy (XPLAN) and then stops.

Less used **OPTIONS:**

--Slow,
Set options to process more accurately.

-p, --project
Set the project name. The default is the prefix taken from
image names. The working directory will be: xds_process_"project"

-d, --distance
Set the detector to crystal distance.

-O, --oscillation
Set frame oscillation range in degree.
For example: -O 0.5

-x, --beam-x
Set a new value for ORGX: X-coordinates (in pixels) of the
detector origin.

-y, --beam-y
Set a new value for ORGY: Y-coordinates (in pixels) of the
detector origin.

-v, --verbose
Turn on verbose output.

-w, --wavelength
Set the x-ray wavelength.

USUAL SESSION:

> **goimg**
> **XDS.py ../col1_1_*.img**
> **less xds_process_col1_1/CORRECT.LP** (look at the high resolution limit)

> **XDS.py -r 1.9 -a -3 -s P3121 -c "59 59 123 90 90 120" ../col1_1_*.img**
> **cd xds_process_col1_1**

> **xscale.py XDS_ASCII.HKL ../xds_process_low/XDS_ASCII.HKL**
> **xdsconv.py XSCALE.HKL 8 Se shelx**
> **xdsconv.py XSCALE.HKL 8 Se solve**
> **xdsconv.py XSCALE.HKL 8 Se ccp4 shelx/XDS_ASCII_F4.hkl**
> **xdsconv.py XSCALE.HKL 8 Se phaser ccp4/XDS_ASCII.mtz**
> **xdsconv.py XSCALE.HKL cns**

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