# XDS.INP input file for data collected on Rigaku FR-X

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!*****************************************************************************
**
! Example file XDS.INP for the PILATUS 200K pixel detector from Rigaku.
! Characters in a line to the right of an exclamation mark are comment.
!*****************************************************************************
**
!==== Often it is necessary to use  MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT=1
!==== DETECTOR PARAMETERS ... PLEASE CHANGE DISTANCE and 2THETA and BEAM
POSITION
!====================== GEOMETRICAL PARAMETERS
==============================

!BEAM POSITION on the detector in pixels is ORGX and ORGY
!ORGX and ORGY are often close to the image center, i.e. ORGX=NX/2,
ORGY=NY/2
ORGX= 207.68 ORGY= 307.84 !Detector origin (pixels).  ORGX=NX/2; ORGY=NY/2

!2theta 0
DIRECTION_OF_DETECTOR_Y-AXIS= 0.0 1.0 0.0
DIRECTION_OF_DETECTOR_X-AXIS= 1.0 0.0 0.0

!2theta 2T
!DIRECTION_OF_DETECTOR_X-AXIS= 0.0 cos(2T) sin(2T)
!DIRECTION_OF_DETECTOR_Y-AXIS= 1.0  0.0 0.0

DETECTOR_DISTANCE= 50   !(mm)

!Other detector stuff probably should be unchanged

DETECTOR=PILATUS         MINIMUM_VALID_PIXEL_VALUE=0  OVERLOAD=1048500
SENSOR_THICKNESS=0.45        !SILICON=-1.0
!AIR=0.001 !Air absorption coefficient of x-rays is computed by XDS by
default
!NX=number of fast pixels (along X); QX=length of an X-pixel (mm)
!NY=number of slow pixels (along Y); QY=length of a  Y-pixel (mm)
!NX=981 NY=1043 QX=0.172  QY=0.172  !PILATUS3 X CdTe 1M
NX=487 NY= 619 QX=0.172  QY=0.172  !PILATUS 300K
!NX=487 NY= 407 QX=0.172  QY=0.172  !PILATUS 200K
!UNTRUSTED_RECTANGLE= 487  495     0 2528
!UNTRUSTED_RECTANGLE=   0 2464   195  213
!UNTRUSTED_RECTANGLE=   0 2464   407  425
UNTRUSTED_RECTANGLE= 0 488 195 213
UNTRUSTED_RECTANGLE= 0 488 407 425
!UNTRUSTED_QUADRILATERAL=565 574  1519 1552  1508 1533  566 1536
!MINIMUM_FRACTION_OF_BACKGROUND_REGION=0.01

TRUSTED_REGION=0.0 1.41 !Relative radii limiting trusted detector region
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!MAXIMUM_NUMBER_OF_JOBS=4  !Speeds-up COLSPOT & INTEGRATE on a Linux-cluster
!MAXIMUM_NUMBER_OF_PROCESSORS=8!<32;ignored by single cpu version of xds
!SECONDS=0   !Maximum number of seconds to wait until data image must appear
!TEST=1     !Test flag. 1,2 additional diagnostics and images

!=== CRYSTAL GONIOMETER which vector was the crystal rotated around?

ROTATION_AXIS= 1.0 0.0 0.0

!====================== JOB CONTROL PARAMETERS
==============================
!JOB= XYCORR INIT COLSPOT IDXREF DEFPIX XPLAN INTEGRATE CORRECT
JOB= XYCORR INIT COLSPOT IDXREF DEFPIX INTEGRATE CORRECT

!=== X-RAY SOURCE PROPERTIES =====  Probably will not change

X-RAY_WAVELENGTH=1.54187           !Angstroem
INCIDENT_BEAM_DIRECTION=0.0 0.0 1.0
FRACTION_OF_POLARIZATION=0.50 !default=0.5 for unpolarized beam
POLARIZATION_PLANE_NORMAL= 1.0 0.0 0.0
!FRACTION_OF_POLARIZATION=0.99 !synchrotron, default=0.5 for unpolarized
beam
!POLARIZATION_PLANE_NORMAL= 0.0 1.0 0.0 ! synchrotron

!=================== SELECTION OF DATA IMAGES
==============================
!Generic file name and format (optional) of data images

NAME_TEMPLATE_OF_DATA_FRAMES=/directory/***.img
!Optimal choice is 0.5*mosaicity (REFLECTING_RANGE_E.S.D.= mosaicity)
OSCILLATION_RANGE=0.10            !degrees (>0)
STARTING_ANGLE=  -90.0
STARTING_FRAME=1
DATA_RANGE=1 1620       !Numbers of first and last data image collected

!BACKGROUND_RANGE=1 6  !Numbers of first and last data image for background

SPOT_RANGE=1 810       !First and last data image number for finding spots

!====================== CRYSTAL PARAMETERS
================================
SPACE_GROUP_NUMBER=0  !0 for unknown crystals; cell constants are ignored.
UNIT_CELL_CONSTANTS=    60 70 80 90 90 90

!You may specify here the x,y,z components for the unit cell vectors if
!known from a previous run using the same crystal in the same orientation
!UNIT_CELL_A-AXIS=
!UNIT_CELL_B-AXIS=
!UNIT_CELL_C-AXIS=
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!Optional reindexing transformation to apply on reflection indices
!REIDX=   0  0 -1  0  0 -1  0  0 -1  0  0  0

FRIEDEL'S_LAW=FALSE !Default is TRUE.

!REFERENCE_DATA_SET= CK.HKL   !Name of a reference data set (optional)
!FIT_B-FACTOR_TO_REFERENCE_DATA_SET=TRUE ! default is FALSE

!==================== DATA COLLECTION STRATEGY (XPLAN)
======================
!                        !!! Warning !!!
!If you processed your data for a crystal with unknown cell constants and
!space group symmetry, XPLAN will report the results for space group P1.

!STARTING_ANGLE=  0.0      STARTING_FRAME=1
!used to define the angular origin about the rotation axis.
!Default:  STARTING_ANGLE=  0 at STARTING_FRAME=first data image

!RESOLUTION_SHELLS=10 6 5 4 3 2 1.5 1.3 1.2

!STARTING_ANGLES_OF_SPINDLE_ROTATION= 0 180 10

!TOTAL_SPINDLE_ROTATION_RANGES=30.0 120 15

!====================== INDEXING PARAMETERS
================================
!Never forget to check this, since the default 0 0 0 is almost always
correct!
!INDEX_ORIGIN= 0 0 0          ! used by "IDXREF" to add an index offset

!Additional parameters for fine tuning that rarely need to be changed
!INDEX_ERROR=0.05 INDEX_MAGNITUDE=8 INDEX_QUALITY=0.8
SEPMIN=4.0       ! default is 6 for other detectors
CLUSTER_RADIUS=2 ! default is 3 for other detectors
!MAXIMUM_ERROR_OF_SPOT_POSITION=3.0
!MAXIMUM_ERROR_OF_SPINDLE_POSITION=2.0
!MINIMUM_FRACTION_OF_INDEXED_SPOTS=0.5

!============== DECISION CONSTANTS FOR FINDING CRYSTAL SYMMETRY
=============
!Decision constants for detection of lattice symmetry (IDXREF, CORRECT)
MAX_CELL_AXIS_ERROR=0.03 ! Maximum relative error in cell axes tolerated
MAX_CELL_ANGLE_ERROR=2.0 ! Maximum cell angle error tolerated

!Decision constants for detection of space group symmetry (CORRECT).
!Resolution range for accepting reflections for space group determination in
!the CORRECT step. It should cover a sufficient number of strong
reflections.
TEST_RESOLUTION_RANGE=8.0 4.5
MIN_RFL_Rmeas= 50 ! Minimum #reflections needed for calculation of Rmeas
MAX_FAC_Rmeas=2.0 ! Sets an upper limit for acceptable Rmeas
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!================ PARAMETERS CONTROLLING REFINEMENTS
======================
!REFINE(IDXREF)=BEAM AXIS ORIENTATION CELL !POSITION
!REFINE(INTEGRATE)=!POSITION BEAM ORIENTATION CELL !AXIS
!REFINE(CORRECT)=POSITION BEAM ORIENTATION CELL AXIS

!================= CRITERIA FOR ACCEPTING REFLECTIONS
=====================
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS= 6000 30000 !Used by DEFPIX
                    !for excluding shaded parts of the detector.

INCLUDE_RESOLUTION_RANGE=50.0 0 !Angstroem; used by DEFPIX,INTEGRATE,CORRECT

!used by CORRECT to exclude ice-reflections
!EXCLUDE_RESOLUTION_RANGE= 3.93 3.87 !ice-ring at 3.897 Angstrom
!EXCLUDE_RESOLUTION_RANGE= 3.70 3.64 !ice-ring at 3.669 Angstrom
!EXCLUDE_RESOLUTION_RANGE= 3.47 3.41 !ice-ring at 3.441 Angstrom
!EXCLUDE_RESOLUTION_RANGE= 2.70 2.64 !ice-ring at 2.671 Angstrom
!EXCLUDE_RESOLUTION_RANGE= 2.28 2.22 !ice-ring at 2.249 Angstrom
!EXCLUDE_RESOLUTION_RANGE= 2.102 2.042 !ice-ring at 2.072 Angstrom - strong
!EXCLUDE_RESOLUTION_RANGE= 1.978 1.918 !ice-ring at 1.948 Angstrom - weak
!EXCLUDE_RESOLUTION_RANGE= 1.948 1.888 !ice-ring at 1.918 Angstrom - strong
!EXCLUDE_RESOLUTION_RANGE= 1.913 1.853 !ice-ring at 1.883 Angstrom - weak
!EXCLUDE_RESOLUTION_RANGE= 1.751 1.691 !ice-ring at 1.721 Angstrom - weak

!MINIMUM_ZETA=0.05 !Defines width of 'blind region'
(XPLAN,INTEGRATE,CORRECT)

!WFAC1=1.0  !This controls the number of rejected MISFITS in CORRECT;
        !a larger value leads to fewer rejections.
!REJECT_ALIEN=20.0 ! Automatic rejection of very strong reflections

!============== INTEGRATION AND PEAK PROFILE PARAMETERS
=====================
!Specification of the peak profile parameters below overrides the automatic
!determination from the images
!Suggested values are listed near the end of INTEGRATE.LP
!BEAM_DIVERGENCE=   0.80         !arctan(spot diameter/DETECTOR_DISTANCE)
!BEAM_DIVERGENCE_E.S.D.=   0.080 !half-width (Sigma) of BEAM_DIVERGENCE
!REFLECTING_RANGE=  0.780 !for crossing the Ewald sphere on shortest route
!REFLECTING_RANGE_E.S.D.=  0.113 !half-width (mosaicity) of REFLECTING_RANGE

NUMBER_OF_PROFILE_GRID_POINTS_ALONG_ALPHA/BETA=13 !used by: INTEGRATE
!NUMBER_OF_PROFILE_GRID_POINTS_ALONG_GAMMA= 9     !used by: INTEGRATE

!DELPHI= 6.0!controls the number of reference profiles and scaling factors
!CUT=2.0    !defines the integration region for profile fitting
!MINPK=75.0 !minimum required percentage of observed reflection intensity
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!======= PARAMETERS CONTROLLING CORRECTION FACTORS (used by: CORRECT)
=======
!MINIMUM_I/SIGMA=3.0 !minimum intensity/sigma required for scaling
reflections
!NBATCH=-1  !controls the number of correction factors along image numbers
!REFLECTIONS/CORRECTION_FACTOR=50   !minimum #reflections/correction needed
!PATCH_SHUTTER_PROBLEM=TRUE         !FALSE is default
!STRICT_ABSORPTION_CORRECTION=TRUE  !FALSE is default
!CORRECTIONS= DECAY MODULATION ABSORPTION

!=========== PARAMETERS DEFINING BACKGROUND AND PEAK PIXELS
================
!STRONG_PIXEL=3.0                                !used by: COLSPOT
!A 'strong' pixel to be included in a spot must exceed the background
!by more than the given multiple of standard deviations.

!MAXIMUM_NUMBER_OF_STRONG_PIXELS=1500000       !used by: COLSPOT

!SPOT_MAXIMUM-CENTROID=3.0                      !used by: COLSPOT

 MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT=1!3        !used by: COLSPOT
!This allows to suppress spurious isolated pixels from entering the
!spot list generated by "COLSPOT".

!NBX=3  NBY=3  !Define a rectangle of size (2*NBX+1)*(2*NBY+1)
!The variation of counts within the rectangle centered at each image pixel
!is used for distinguishing between background and spot pixels.

!BACKGROUND_PIXEL=6.0                           !used by: COLSPOT,INTEGRATE
!An image pixel does not belong to the background region if the local
!pixel variation exceeds the expected variation by the given number of
!standard deviations.

!SIGNAL_PIXEL=3.0                               !used by: INTEGRATE
!A pixel above the threshold contributes to the spot centroid

!DATA_RANGE_FIXED_SCALE_FACTOR= 1 60 1.0 ! used by : INIT,INTEGRATE
```