

**XDS.INP input file for data collected on Rigaku FR-X with EIGER 4M**

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! Example file XDS.INP for the EIGER 4M pixel detector, IGBMC CBI
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! Last edit: Alastair McEwen, 2017/07/06
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!===== JOB CONTROL PARAMETERS
=====!
JOB= XYCORR INIT COLSPOT IDXREF DEFPIX INTEGRATE CORRECT
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  MAXIMUM_NUMBER_OF_PROCESSORS=4

!===== GEOMETRICAL PARAMETERS
=====!
  ORGX=1010.21  ORGY=831.47      !Detector origin (pixels)
  DETECTOR_DISTANCE= 61        !(mm) (range = 61 - 280)
  OSCILLATION_RANGE=0.25      !degrees (>0)
  X-RAY_WAVELENGTH=1.54178    !Angstroem (do not change)
  STARTING_ANGLE=-68          !degrees

!===== CRYSTAL PARAMETERS
=====!
  SPACE_GROUP_NUMBER=0      !0 for unknown crystals; cell constants are ignored.
  UNIT_CELL_CONSTANTS= 77.7 77.7 77.7 90 90 90
!REIDX=  0  0 -1  0  0 -1  0  0 -1  0  0  0
  FRIEDEL'S_LAW=FALSE !Default is TRUE

!===== SELECTION OF DATA IMAGES
=====!
  NAME_TEMPLATE_OF_DATA_FRAMES=path-to/Image_????.img
  STARTING_FRAME=101        !Number of first image
  DATA_RANGE=1 720        !Numbers of first and last data image collected
!BACKGROUND_RANGE=1 40    !rather use defaults (first 5 degrees of rotation)
  SPOT_RANGE=1 360        !First and last data image number for finding spots
!REFERENCE_DATA_SET=./XDS_ASCII.HKL

!===== PARAMETERS CONTROLLING REFINEMENTS
=====!
  REFINE(IDXREF)=CELL BEAM ORIENTATION AXIS !DISTANCE POSITION
  REFINE(INTEGRATE)=DISTANCE POSITION BEAM ORIENTATION ! AXIS CELL
!REFINE(CORRECT)=CELL BEAM ORIENTATION AXIS DISTANCE POSITION !Default is:
refine everything
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!===== DETECTOR AND GENERATOR PARAMETERS
=====!
DETECTOR=EIGER
MINIMUM_VALID_PIXEL_VALUE=0 OVERLOAD=2147483647
SENSOR_THICKNESS=0.45
NX=2070 NY=2167 QX=0.075 QY=0.075
DIRECTION_OF_DETECTOR_X-AXIS=0.927184 0 0.374607 !cos(2theta) 0 sin(2theta)
DIRECTION_OF_DETECTOR_Y-AXIS=0.0 1.0 0.0
ROTATION_AXIS=0 -1 0
INCIDENT_BEAM_DIRECTION=0.0 0.0 1.0
POLARIZATION_PLANE_NORMAL=1 0 0
FRACTION_OF_POLARIZATION=0.50 !default=0.5 for unpolarized beam
TRUSTED_REGION=0.0 1.2 ! partially use corners of detector (0 1.4143: use
all pixels)

UNTRUSTED_RECTANGLE= 1030 1041 0 2168
UNTRUSTED_RECTANGLE= 0 2071 514 552
UNTRUSTED_RECTANGLE= 0 2071 1065 1103
UNTRUSTED_RECTANGLE= 0 2071 1616 1654

!===== INDEXING PARAMETERS
=====!
STRONG_PIXEL=4 ! COLSPOT: only use strong reflections (default is
3)
MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT=3 ! default of 6 is sometimes too high

!===== 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

!===== 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 1.5 !Angstroem; used by
DEFPIX, INTEGRATE, CORRECT

!used by CORRECT to exclude ice-reflections
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!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
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!===== INTEGRATION AND PEAK PROFILE PARAMETERS
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NUMBER_OF_PROFILE_GRID_POINTS_ALONG_ALPHA/BETA=13!used by: INTEGRATE
!NUMBER_OF_PROFILE_GRID_POINTS_ALONG_GAMMA= 9 !used by: INTEGRATE
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cbi-eiger-4m-xds-v1.inp

pilatus300k\_frx\_xds.inp

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