

Protein Crystallography

A simple, reactor-based example instrument for MX diffraction is the instrument file <http://trac.mccode.org/browser/trunk/mcstas-comps/examples/templateNMX.instr> of the McStas distribution.

Also see [\[Generating a new Laue file\]](#)

A snapshot of the contents dating from early 2015 is provided below and shows example use of

- The Single_crystal component
- SPLIT for boosting simulation stats

For the Rubredoxin.lau system, the Single_crystal component has suggested to use a SPLIT repetition number of 43, corresponding to the average number of active reflections in the system. That chosen split value will give you an efficiency factor of 43 in production of reflected neutrons from the sample.

```
/* *****  
* McStas instrument definition URL=http://www.mcstas.org  
*  
* Instrument: templateLaue  
*  
* %Identification  
* Written by: K. Nielsen  
* Date: June 2nd, 2010  
* Origin: ILL  
* Release: McStas CVS-080208  
* Version: $Revision: 5074 $  
* Modified by: EF, PW  
* %INSTRUMENT_SITE: Templates  
*  
* A simple Laue NMX diffractometer for macromolecules, adapted from the classic  
* templateLaue instrument.  
*  
* %Description  
* A single crystal sample is illuminated with a white cold beam.  
* Based on a Laue tutorial written by K. Nielsen, Feb 7, 2000.  
*  
* Example: templateNMX REPS=50 reflections=Rubredoxin.lau Detector: det_I=210.788  
* Example: templateNMX REPS=700 reflections=PPase_D_P1.lau Detector: det_I=29.6512  
*  
* %Parameters  
*  
* %End  
*****/  
  
/* Change name of instrument and input parameters with default values */  
DEFINE INSTRUMENT templateNMX(REPS=43, string reflections="Rubredoxin.lau")  
  
TRACE  
  
COMPONENT Origin = Progress_bar()  
  AT (0,0,0) ABSOLUTE  
  
COMPONENT source = Source_simple(  
  radius=0.02, focus_xw=0.001, focus_yh=0.001,  
  lambda0=7, dlambda=5, flux=1e12)  
AT (0,0,0) ABSOLUTE  
  
COMPONENT slit = Slit(  
  xwidth=0.001, yheight=0.001)  
AT (0,0,5) RELATIVE source  
  
SPLIT REPS COMPONENT sample = Single_crystal(  
  xwidth=0.001, yheight=0.001, zdepth=0.001, mosaic=1e-3,  
  reflections=reflections)  
AT (0,0,0.10) RELATIVE slit  
EXTEND %  
  if (!SCATTERED) ABSORB; /* perfect beam stop */  
%}  
  
COMPONENT det= PSD_monitor_4PI(radius=1, nx=360,ny=180,filename="psd")  
AT (0,0,0) RELATIVE sample  
  
END
```