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<pre> import sys import iotbx.mtz sys.path.append("/Users/kuntaro/00.Develop/Prog/02.Python/Libs/") from ReflWidthBothEdge import * #### # One liner function for extracting Intensity related columns in MTZ file #### get_I_arrays = lambda x: filter(lambda y: y.is_xray_intensity_array(), x) def run(ref_mtz, frame_mtz, matfile): ##### # MTZ file reading ##### ref_arrays = iotbx.mtz.object(ref_mtz).as_miller_arrays() frame_arrays = iotbx.mtz.object(frame_mtz).as_miller_arrays() ##### # Obtain all of the symmetry operation from FRAME MTZ ##### ops = [op.inverse().r() for op in iotbx.mtz.object(frame_mtz).space_group().all_ops()] ##### # Intensity related cctbx.array ##### ref_I = get_I_arrays(ref_arrays)[0] frame_I = get_I_arrays(frame_arrays)[0] m_isym = filter(lambda a: "M_ISYM" in a.info().labels, frame_arrays)[0] print "Selected refl:", ref_mtz, ref_I.info().label_string() print "Selected frmI:", frame_mtz, frame_I.info().label_string() print "Selected M/ISYM:", frame_mtz, m_isym.info().label_string() # Take common sets of these ref_I, frame_I = ref_I.common_sets(frame_I, assert_is_similar_symmetry=False) m_isym, ref_I = m_isym.common_sets(ref_I, assert_is_similar_symmetry=False) m_isym, frame_I = m_isym.common_sets(frame_I, assert_is_similar_symmetry=False) ##### # delete FULL/PARTIAL flag ##### isyms = m_isym.data()%256 # Preparation for diffraction width rwbe=ReflWidthBothEdge(matfile,0.02,0.02,0.3,0.0002,0.1) for (hkl1, rI, rsigI), (hkl2, fI, fsigI), isym in zip(ref_I, frame_I, isyms): assert hkl1 == hkl2 # Calculate original index sign = -1 if isym%2 == 0 else 1 ohkl = hkl1*ops[int((isym-1)/2)] ohkl = tuple(map(lambda x:int(x*sign), ohkl)) rwbe.setHKL(ohkl,0.0) rwbe.calcDELEPS() pcalc=rwbe.calcPartiality() #print hkl1, ohkl, rI, fI,pcalc pobs=fI/rI print "%12.6f%12.6f"%(pobs,pcalc) #print ohkl, rI, fI,pcalc </pre>		

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<pre> print "Done." if __name__ == "__main__": ref_mtz = sys.argv[1] frame_mtz = sys.argv[2] mat_file=sys.argv[3] run(ref_mtz, frame_mtz, mat_file) </pre>		