

Sep 15, 12 18:14

MtzRefl.py

Page 1/1

```
import iotbx.mtz
from cctbx.array_family import flex
import sys, os, math
from ReflWidth import *
from ReadMtz import *

if __name__=="__main__":
    if len(sys.argv)!=3:
        print "Usage MTZFILE MATFILE"
        sys.exit()

    mtzf=ReadMtz(sys.argv[1])
    refl=mtzf.getOriginalIndex()
    rw=ReflWidth(sys.argv[2],0.02,0.02,0.3,0.0002,0.1)

    for hkl in refl:
        if rw.setHKL(hkl)==True:
            rw.calcDELEPS(0.0)

    #print type(test)
    #test2=array(test)
    #for hkl in test2:
        #print "HKL",type(hkl)
        #if rw.setHKL(hkl)==True:
            #rw.solvePhi(0.0)
            #rw.distESToRLP()
            #rw.calcLorentz()
            #rw.calcRspot()
            #rw.diffWidth()
            #rw.cuspcheck()
            #rw.calcDELEPS()
```