1 Introduction

This document describes what is needed to make a wrapper for the CCP4 program reindex. This is used to map reflection indices from one spacegroup, most useful when an integrated data set is found to be indexed in the wrong pointgroup or setting.

1.1 Background

The most likely case where this would be used is in response to a run of pointless. The possible cases for this are:

- Solitary data set - indexing to the correct pointgroup.

- Matching a moving data set to a reference set.

- Correctly assigning the spacegroup in the file header.

Combinations of these are also likely. An example of a reindex command script is:

```
#!/bin/bash
reindex HKLIN 12287_1_E1_.mtz HKLOUT 12287_1_E1_scaled_reindex.mtz << eof
SYMMETRY 'P 4 2 2'
REINDEX h, k, l
eof
```

The correct symmetry and reindexing operator will come from pointles, though by specifying a HKLOUT file it is possible to simply use pointless for this. However, this may be useful when a user has provided the "correct" spacegroup or something.

2 Use Cases

2.1 Use Case 1: Reindexing to a provided spacegroup

This presumes that you simply want to change the spacegroup label in the reflection file but not change the reflection indices. This is correct for changing from tetragonal spacegroup P4 to say P422. The JCSG dataset 1VPJ illustrates this well.

2.2 Use Case 2: Reindexing with a provided reindexing operator

If you have a spacegroup like P23 where alternative indexings are possible, it may be necessary to perform the reindexing to ensure that the resulting reflections match up correctly. One of Ed Mitchell's data sets illustrates this well - whichever one is cubic.