

# EMSFREF.DOC

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## A. INTRODUCTION

EMSFREF is an "all-purpose" program for refining structure factor data. This program is NOT for the WEAK-AT-HEART. If you are not certain what you are doing, this program is SURE to ruin what may have been a decent set of data. In other words, USE AT YOUR OWN RISK. It has been said many times by others that "there is no such thing as a debugged program". "They", of course, are correct. Thus the management would appreciate any help with tracking down those elusive creatures.

## B. PROGRAM OPTIONS

TOUCH-KEY options available include:

- (C) Shift phase origin
- (D) Change SF data to rotate or flip 'IMAGE'
- (F) Compare phase origins for 2 SF files
- (G) Combine two or more SF data sets
- (H) Apply a scale factor to the SF data
- (I) Change SFs to invert contrast in 'IMAGE'
- (J) Compute a linear scale factor between two SF data sets
- (K) Convert from SF file format to EMSFZLNE compatible format
- (E) EXIT program

### **OPTION D: Change SF data to rotate or flip 'IMAGE'**

This option will alter the SF data to cause a rotation by 180 degrees or an inversion (changing the hand) about a vertical mirror line of the reconstruction MAP. Note: at present, this option ONLY works for ORTHOGONAL or HEXAGONAL plane groups.

### **OPTION F: Compare phase origins for 2 SF files**

**NOTE: THIS OPTION IS NOT CURRENTLY AVAILABLE !!!!!**

This is used to determine the absolute phase shift between two SF data sets. The first data set is compared to the second (reference) data set.

**OPTION G: Combine two or more SF data sets**

This option can be used to add two or more SF data sets together. Note that by scaling one set with a negative scale factor, you can compute a SF data set which will produce a difference MAP.

There are two ways in which the combined data may be scaled. The merged SF data are either divided globally by the number of data sets read in, or each SF measurement is scaled according to the number of common measurements. The first option will downweight those SF data with fewer overlaps. This is advised for merging data sets which ought to contain equivalent sets of hkl data. The second option is advised for merging data sets which are known to contain SF measurements that are not found in all the data sets.

**OPTION I: Change SFs to invert contrast in 'IMAGE'**

180 degrees is added to each phase. The effect of this is to reverse the contrast in the back-transformed reconstruction.

**OPTION J: Compute a linear scale factor between two SF data sets**

This will compare the SF data from two data sets and report a linear scale factor based on NTOT SF comparisons. Two R-factor measurements are given, the first based on amplitudes only and the second based on the REAL and IMMAGINARY Fourier components.

**OPTION K: Convert from SF file format to EMSFZLNE compatible format**

This will take the data from a standard SF file and convert it into the EMSFZLNE program compatible format. The main intent of this option is to allow the user to plot SF measurements from truncated 3D MAP data obtained from the reconstruction of a tilt series using the EMSFZLNE program software.