

# EMICOSYM.DOC

(last update Dec 10, 1990)

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### A. INTRODUCTION

EMICOSYM imposes 3-fold symmetry on a 3D MAP. The program is typically run after EMICOFB, which only produces a 3D MAP of the icosahedral particle with strict 522 symmetry. EMICOSYM generates a 3D reconstruction MAP with full 532 icosahedral symmetry. This program was adapted from SYMMETRIZE, written by S. Fuller (Heidelberg).

### B. PROGRAM INPUT

1. INPUT FILENAME (A)
2. OUTPUT FILENAME (A; DEFAULT=EMICOSYM.MAP)
3. HEADER (18A4; DEFAULT=old header)
4. NCOL2,NROW2,NSEC2 (3I; DEFAULT=old NCOL,NROW,NSEC)

1. INPUT FILENAME (A)

-----

Specifies the name of the input 3D MAP file.

2. OUTPUT FILENAME (A; DEFAULT=EMICOSYM.MAP)

-----

Specifies the name of the symmetrized output 3D MAP file.

3. HEADER (18A4; DEFAULT=old header)

-----

Use a header, for example, to identify the symmetrized 3D MAP.

4. NCOL2,NROW2,NSEC2 (3I; DEFAULT=input 3D MAP dimensions)

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These specify the desired dimensions of the output 3D MAP.

### C. PROGRAM EXECUTION

On Purdue's VAX 8550, it takes about 3 minutes to process a

100x100x100 3D MAP (input same size as output). A 200x200x200 3D MAP (eight times larger volume) takes about 24 minutes to process.

#### **D. FINAL NOTES**

1. [TSB.FOR]EMICOSYM.BCH contains an example BATCH job command file for running EMICOSYM.

```
=====
==
FORTRAN code:  DEXTRO3:[TSB.FOR]EMICOSYM.FOR.
Documentation: DEXTRO3:[TSB.FOR.DOC]EMICOSYM.DOC          10-Dec-90
-----
--
```

## E. FLOW CHART FOR EMICOSYM PROGRAM

```
*****
*           MAIN           *
* (EMICOSYM.FOR)        *
*****
*
*-- GET_3F_MATRIX - GENROT
*
*-- OPEN_INITIAL - MAP_OPEN -- |-- STRING_UPPER
*                               |-- FILE_CHECK
*-- MAPI2_FILL_3D
*
*-- OPEN_OUTPUT - STRING_UPPER
*
*-- CALCULATE_EQUIVALENTS - VECMUL
*
*-- REMOVE_OVERLAPS
*
*-- GET_EQUIVALENT_VALUES - INTERP3D
*
*-- FILL_PERP2
*
*-- MAPI2_WRITESEC
```