EMICOROT.DOC

(last update Dec 10, 1990)

CONTENTS

A. INTRODUCTION

EMICOROT is used to rotate a 3D MAP of an icosahedral particle
(MUST be in the standard 2-fold orientation: see
[TSB.DOC]EMICO_SYS.DOC) to any equatorial (THETA=90) view. This
program is adapted from the original MRC routine ROTATE3.
EMICOROT is generally run after EMICOFB (or EMICOSYM). Note that
this program is not strictly restricted to working with 3D MAPs of
icosahedral particles, however, such rotations are typically
carried out with EMMAP (option "R") which is not just restricted
to the generation of equatorial orientations.

B. PROGRAM INPUT

1. INPUT FILENAME (A)
2. OUTPUT FILENAME (A; DEFAULT=EMICOROT.MAP)
3. HEADER (18A4)
4. PHI (F; DEFAULT=0.0, the two-fold view)
5. NHAND (I; DEFAULT=0)
6. DENS (F; DEFAULT=0.0)

1. INPUT FILENAME (A)

   This specifies the input 3D MAP file.

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

   The name of the file which stores the rotated 3D MAP.

3. HEADER (18A4)

   A header may be used, for example, to identify the data.

4. PHI (F; DEFAULT=0.0, the two-fold view)

   PHI selects the desired equatorial view. For example, PHI =

31.7174 gives the 5-fold view, and PHI = 69.0948 gives the 3-fold view.

5. NHAND (I; DEFAULT=0)

   If NHAND = 1, the output 3D MAP will have the hand reversed relative to the input 3D MAP. Any other value for NHAND will leave the MAP hand unchanged.

6. DENS (F; DEFAULT=0.0)

   This specifies the density value substituted for every voxel outside the spherical envelope with a diameter = NCOL.

C. PROGRAM EXECUTION

   The program attempts to perform all calculations in the computer core memory. If sufficient core memory is unavailable, scratch disk space is used. The in-core version runs much faster than the I/O bound version.

D. FINAL NOTES

1. Examples of BATCH job command files for creating 3D MAPs in either the 3-fold or 5-fold orientations are given in [TSB.FOR]EMICOROT_3F.BCH and [TSB.FOR]EMICOROT_5F.BCH.

2. As a possible future option, the program may be revised to allow output of only a partial 3D MAP to save computations and space.

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

E. FLOW CHART FOR EMICOROT PROGRAM

```
*****************
*      MAIN      *
* (EMICOROT.FOR) *
*****************
        *
        *-- MAP_OPEN --|-- STRING_UPPER
        *              |-- FILE_CHECK
        *-- PIRADDEG
        *
        *-- ICO_ROTATE_FAST
        *
        *-- ICO_ROTATE_SLOW - MAP_HEADER
```