

MBLDSF.DOC

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A. INTRODUCTION

MBLDSF is a model building program which produces a file of structure factor data (2D or 3D). The user sets up a control data file defining rotational and/or crystallographic symmetry operators and identifying the atoms (size, shape and position). Structure factor data for any atomic crystal structure can be produced within certain limits (# atoms = 1500, # structure factors = 50,000). All distances measured in nms.

A model structure is constructed by defining the location, size and shape for all the atoms within the asymmetric unit of the structural motif. The motif is then generated by applying the rotational symmetry operator(s) and the crystal structure is generated by applying the crystallographic symmetry operator(s). The format for setting up the control data parameters appears below.

To run the program first type the name of the file containing the control parameters, then enter a name for storing the output structure factor data (and a header identifier if desired). If you wish to apply a temperature factor to the SF data, enter the resolution at which data is multiplied by 1/exp.

B. FORMAT FOR CONTROL PARAMETER DATA FILE

CARD	DESCRIPTION
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(1)	SF_TITLE (18A4) Header record for SF data file.
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(2)	A_CELL,B_CELL,C_CELL,ALP,BET,GAM,RESHI,RESLO (8F)
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A_CELL,B_CELL,C_CELL	= cell dimensions in nms.
ALP,BET,GAM	= cell angles in degrees.
RESHI	= high resolution limit in nms.
RESLO	= low resolution limit in nms (if negative, the origin SF (F0) will be computed).

(3) NROT,NCRYST,SCALE (2I,F)

NROT = number of rotational symmetry operators.

NCRYST = number of crystallographic operators.

SCALE = scale factor for structure factors.

(4) MAXH,MINH,MAXK,MINK,MAXL,MINL (6I)

Miller indices limits. This is another way, along with RESHI and RESLO to limit the range of SF data computed. A SF is calculated only if both tests are passed.

(5->4+NROT) PSI,FI,KAPPA (3F) Defines the location and symmetry of each symmetry operator.

PSI = angle in the xy plane measured + from y --> x.

FI = angle in the xz plane measured + from x away from z.

KAPPA = rotational angle.

(5+NROT) PSI,FI,ANGLE (3F) Same as above, for skewing the motif.

(6+NROT->6+NROT+NCRYST) T(NCRYST,3,4) (12F) Defines the general positions in the unit cell (one for each crystallographic operator).

As an example, consider the case of space group P2(1)2(1)2. If you look on page 104 of the International Tables for X-ray Crystallography (19??) you will see that the coordinates of the four equivalent positions are:

$x, y, z; -x, -y, z; 0.5+x, 0.5-y, -z; \text{ and } 0.5-x, 0.5+y, -z$

These would be entered in the control file as four records:

```
1., 0., 0., 0., 0., 1., 0., 0., 0., 0., 1. 0.
-1., 0., 0., 0., 0., -1., 0., 0., 0., 0., 1. 0.
1., 0., 0., .5, 0., -1., 0., .5, 0., 0., -1. 0.
-1., 0., 0., .5, 0., 1., 0., .5, 0., 0., -1. 0.
```

(7+NROT+NCRYST) TRANS(3) (3F) Fractional position of the origin of the motif in the unit cell.

(8+NROT+NCRYST) NATOS (I) The number of atoms in the asymmetric unit of the motif.

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(9+NROT+NCRYST->?) ANUM,PSI,FI,R,B,TYPE,ICRYST,ICART (6F,2I)
One for each atom.
ANUM      = atom weight.
PSI,FI,R  = spherical polar coordinates (if ICART = 0).
           Cartesian coordinates (x,y,z in nms if ICART
           = 1).
B         = atom radius in nms.
TYPE      = 1.0 for Gaussian; = 2.0 for hard sphere atom
           shape.
ICRYST    = 0: Apply rotational and crystallographic
           operators.
           1: Apply crystallographic operator(s) only.
ICART     = see PSI,FI,R.

```

An example of a control data file appears below:

```

PENTAMER MODEL
10.0, 10.0, 10.0, 90., 90., 90., 2.0, -1000.
1, 1, 1.0
31, -31, 31, -31, 31, 0
90., 90., 72.
90., 90., -5.0
1.,0.,0.,0., 0.,1.,0.,0., 0.,0.,1.,0.
0.5, 0.5, 0.5
1
100., 0., 2.8, 0., 1.5, 2., 0., 0, 1

```

This produces a pentamer model (5 total atoms) in a 10x10x10 nm cubic unit cell. Structure factors are computed out to a resolution of 2.0 nm. There is one rotational symmetry operator and one (the identity) crystallographic operator. The scale factor = 1.0. The Miller indices restrictions will not allow structure factors to be calculated with $L < 0$. WARNING: The program automatically screens for and deletes any Friedel mates or duplicate structure factor data. There is a 5-fold (rotational angle = 72.0) symmetry axis coincident with the z-axis. The motif (a pentamer) is rotated by 5 degrees counterclockwise about the z-axis direction. The only crystallographic operator is the identity operator (i.e. there is no crystallographic symmetry in this crystal model). The motif is positioned at the center (fractional coordinates = 0.5,0.5,0.5) of the unit cell. The one atom which is operated on by the 5-fold symmetry axis and the identity operator has a weight of 100 and is positioned at $x,y,z=0.,2.8,0.$ (in Cartesian coordinates, in nms). The atom is 1.5 nm in radius and has a hard spherical shape.

NOTE: The file MBLDSF.TMP, a byproduct of this program, contains the x,y,z coordinates of the "atoms" in the model. This

file can be used with the program PLTMOD to plot "stick" drawings of the model.

PLTMOD is a "quick-and-dirty" program, originally designed to just plot diagrams of icosahedra. It could be modified quite easily to provide fancier plots (i.e. perspectives, hidden lines, etc.).