Chapter 3

XDINI – Importing Data into XD

XDINI provides an interface between XD and certain crystallographic computer packages used to solve and refine the structure. It creates the master file with default options and settings, the corresponding input-parameter (`xd.inp`) and data files (`xd.hkl`) for XDLSM. An output file (`xd_ini.out`) is also written. The program either requires keywords given in the command line or input from the file `xd_ini.inp`. The current version supports data transfer from SHELX (SHELXTL), CIF and XTAL files. It also accepts free-format, as well as fixed-format data files, making it possible to communicate with other computer packages. The files created by XDINI need to be checked. The default setting corresponds to a spherical-atom refinement. It is necessary to edit and modify the **ATOM** table in the master file before switching to multipole refinement. The default definition of the atomic site coordinate systems are based on the connectivity (the two closest neighbours together with the atom considered define the Z,X plane). This is, in most of the cases, not appropriate for site symmetry implementations. The level of the multipole expansion (the default is monopole) as well as the number of kappa sets should be extended. The `xd.inp` and `xd.hkl` files usually do not need to be modified.

3.1 Instructions for XDINI

3.1.1 Command line mode

In the command-line mode, no `xd_ini.inp` file is required. The following simple syntax can be used:

xdini *cid prgname bnkname*
(e.g. `xdini test shelx SCM`)

cid is a maximum 8 character long compound identification described before and *prgname* can be **shelx**, **cif** and **xtal** with the following input-file requirements:

prgname	file1	file2	file3
shelx	`shelx.ins`	-	`shelx.hkl`
cif	`xd.cif`	-	`xd.fcf`
xtal	`xtal.inp`	`xtal.stm`	`xtal.hkl`

The files file1-3 are read, each after the other, in the order given above. If any of them is not found or its interpretation failed, XDINI turns to its standard input file, `xd_ini.inp`, for further instructions. *bnkname* can be CR, BBB, SCM or VM (see section 2.5 for their meaning). If *bnkname* is not specified, `xd.mas` will be generated with the default BANK CR.

If cif format files are used as input, it is *essential* that the data_ block name is identical in both the parameter and reflection data files, *i.e.* both must have the same ***data_<name>*** at the start of the file (note that ***<name>*** is case insensitive).

3.1.2 File directed mode

xdini *cid*
The input file (`xd_ini.inp`) consists of three segments: general crystallographic, parameter and observation input. The first one corresponds to that in the master file containing the instructions **TITLE**, **CELL**, **SYM**, **LATT**, **BANKFILE** and **WAVE**, among which the first two always have to be given. The latter two segments have common instructions described below.

3.1.3 FILE

FILE *filename*

The data are read from the input file `xd_ini.inp` unless otherwise is specified. The **FILE** instruction redirects the default input to a file named *filename*.

3.1.4 FORMAT

FORMAT (*format specification*)

The data are supposed to be given in default order and in free format. If this is not the case a proper format instruction (standard FORTRAN) is to be given. The format specification in parentheses must be divided by a blank from the **FORMAT** command.

3.1.5 Default atomic parameter list

The following entries have to be given for each atom:

atomname x y z mult uiso or
u11 u22 u33 u12 u13 u23

The *atomname* (up to eight characters) should start with a proper element symbol followed by any character string. It is transformed to the atom identifier standard to XD (NA11 to Na(11) or h2a to H(2a)). *x*, *y* and *z* are fractional coordinates corresponding to the cell dimensions given by the **CELL** card. The last two entries, the atomic site occupation factor (*mult*) and the isotropic thermal parameter (*uiso*) can be omitted if the atom is in general position and anisotropic displacement parameters are supplied in the next line.

3.1.6 LOADPAR

LOADPAR *nat (npar)*

Followed this command line *nat* atom segments are read. The parameters have to be either in the order specified above or according to a format statement given previously. In the latter case the number of entries (including *atomname*) for each atom has to by given by *npar*.

3.1.7 DTYP

DTYP u|b|beta

This instruction specifies the type of the displacement parameters in the atom line. A general expression for the anisotropic atomic thermal parameter is

$$t = \exp\left(-\sum_{ij} d_{ij} A_{ij} \right) \quad \text{with } i \geq j = 1, 2, 3$$

For the three options above the constants (d_{ij}) and the displacement amplitudes (A_{ij}) take the following forms:

dtyp	d_{ij}	A_{ij}
u	$2\pi^2 a_i a_j h_i h_j (2 - \delta_{ij})$	U_{ij}
b	$a_i a_j h_i h_j (2 - \delta_{ij})$	$B_{ij} = 8\pi^2 U_{ij}$
beta	$h_i h_j (2 - \delta_{ij})$	$b_{ij} = 2\pi^2 a_i a_j U_{ij}$

where

$$\delta_{ij} = \begin{cases} 1 \text{ for } i = j \\ 0 \text{ for } i \neq j \end{cases}$$

a_i are reciprocal axis lengths and h_i are the corresponding components of the scattering vector.
If the input displacement amplitudes are in the form of **b** or **beta** they are transformed to **u** as required by XDLSM.

3.1.8 SCALE

SCALE *(sc(i),i=1,nsc) [1.0]*
nsc number of scale factors are read in. If omitted the data are supposed to be on absolute scale forming one scale group.

3.1.9 Default observation input

The following entries can be given for each observation:

h k l obs sigobs scgrp tbar u1 u2 u3 v1 v2 v3

These symbols are described in the previous chapter in connection with the reflection file `xd.hkl`. The first 5 entries always have to be given, all others are optional.

3.1.10 LOADREF

LOADREF F or **F^2** *nref ndat*
nref observation line, containing *ndat* entries with *F* or F^2 data, are read either in the order specified above or according to a format statement given previously.

3.1.11 SORT

SORT (*index1* [**h**] *index2* [**l**] | **sinthl**)

The reflections are sorted either with respect to indices (*index1* varies first and *index2* last) or to the absolute value of the scattering vector (**sinthl**). An in-memory sorting algorithm is implemented which can handle 15000 reflections. If more data are to be sorted, the parameter NO has to be changed in the source. Proper sorting with respect to indices speeds up the Fourier calculations. It is mentioned here that XDINI does not average symmetry equivalent reflections and neither does XDLSM. It is advised to enter into XD with unique (symmetry-averaged) data unless anisotropic extinction refinement is to be carried out.

3.1.12 END

END

The **END** card closes the `xd_ini.inp` file and terminates the program.

3.2 Examples

Example 1.

```
TITLE oxal    (free format atom list)
CELL  6.093 3.469 11.9257 90. 105.69 90.
SYMM 1/2-X, 1/2+Y, 1/2-Z
LATT C P
SCALE  3  85.87513 89.84698 369.09409
LOADPAR 7
O1     0.085335 -0.055242 0.150354
 0.006503 0.009821 0.003786 0.002344 0.001042 0.000470
O2    -0.221518 0.244985 0.036284
 0.005563 0.009277 0.005550 0.002939 0.001704 0.000386
O3    -0.451596 0.634692 0.178431
 0.006991 0.009768 0.005222 0.001231 0.002255 0.000790
 ...
H3    -0.373817 0.487426 0.152675 1.0 0.03
FILE   ox.hkl
LOADREF  1500 6
SORT  sinthl
END
```