

Chapter 2

The XD System Files and the Master Control Program

2.1 File Name Conventions

The xd files are named according to the convention

$$\text{xd}(\text{_model-ID})(\text{_property} \mid \text{_program}).\text{_type}$$

The prefix *xd* serves to distinguish the file as an XD system file from others that the user may want to keep in the same directory. The fields in parentheses are optional.

2.1.1 The Model-ID Field

The *model-ID* field can be used to distinguished different refinement models. It is applied to the parameter file and related files only when the model-ID is specified on the command line (cf. Section 2.11).

2.1.2 The Property Field

The *property* field refers to the property used for the calculations. It is mainly used for grid files and output from the property program.

rho	electron density
defden	deformation density
gradrho	gradient of the electron density
d2rho	Laplacian
esp	electrostatic potential
fou	Fourier map
fft	Fourier map
core	core density
valence	valence density
nucpot	nuclear potential
sigrho	error of the electron density
siglap	error of the Laplacian
oep	one electron potential
elf	electron localisation function (using Kirzhnitz approximation)
nci	reduced electron density gradient (Non Covalent Interactions)
dori	density overlap regions indicator
sedd	single exponential decay detector
rhos	electron density multiplied by the sign of λ_2 of Hessian
ked	kinetic energy density (using Kirzhnitz approximation)
ped	potential energy density (using Kirzhnitz approximation)
ted	total energy density (using Kirzhnitz approximation)
eig2	second eigenvalue of electron density Hessian - similarly eig1 eig3

2.1.3 The Program Field

The *program* field specifies the program which created the file. *program* can be ini, lsm, pro, geom, fft or fou.

2.1.4 The File Type

The file *type* can be one of the following : (a * marks files for which the *model-ID* can be used; filenames for which the *property* field is applied are marked with a †, while those which make use of the *program* field are marked ‡)

mas	the master file
cyc	cycle information
hkl	reflection data
out*†	list-able output
inp*	see res
res*	all atomic and all refinable parameters
fou*	Fourier file (binary)
cov*	variance-covariance matrix (binary)
der*	matrix of structure factors derivatives (binary)
mat*	normal equation matrix (binary)
grd*†	property on a grid
pth*	bond path
cps*†	critical points
ps†	PostScript graphical output
hpg†	HPGL graphical output
cgm†	CGM (Computer Graphics Metafile) graphical output

2.1.5 Examples of File Names

xd.mas	(master file)
xd_lsm.out	(least squares results listing)
xd.res	(least squares parameter file on output)
xd.fou	(Fourier reflection file)
xd.cov	(variance-covariance matrix)
xd_defden.grd	(deformation density on a grid)

2.1.6 The Cycle Field and the Cycle File

The *cycle* field is applied only in case the file `xd.cyc` is present. In this case it is used to add cycle (version) numbers to the `.res` file. XDLSM usually reads from `xd.inp` and writes to `xd.res`. The cycle file contains instructions about the cycle to read and the first cycle to write. It consists of the single line

READ *rdcyc* **WRITE** *wrcyc*

If the read cycle equals zero, `xd.inp` is read. If the write cycle equals zero, the behaviour is undefined. After each refinement cycle, XDLSM sets *rdcyc* to *wrcyc* and increments *wrcyc* by one. After the last cycle, the new values are written to `xd.cyc`. When XDLSM is run again, it reads the last parameter file written and continues to write new parameter file following the existing ones. In case XDLSM dies before finishing the last cycle, no new cycle file is written and possibly created parameter files of this run are ignored.

In case the cycle naming scheme is to be used, one starts with **READ** 0 **WRITE** 1 after XDINI has run. There is no need to touch the cycle file after that if things go right. To restart the refinement from a specific cycle, edit the **READ** field. The **WRITE** field only needs to be

edited if parameter files should be overwritten after a successful run of XDLSM or, conversely if parameter files should not be overwritten after an unsuccessful run.

Note, that the cycle mechanism is only available on platforms which support multiple periods in file names (Unix/Linux and Windows all accept this mechanism).

2.2 The Master File **xd.mas**

Execution of the component programs of the XD package is started by a master control program directed by a master file. **xd.mas** is a free-format ASCII file. A line beginning with the exclamation mark (!) will be treated as a comment. This allows the user to keep all instructions in the file even if many of them are not in actual use. A single line can have up to 256 characters. If a line ends with a forwardslash (\), the next line will be read as a continuation line. The total length of a concatenated lines can be up to 256 characters. The input is *not* case sensitive. Two special tokens, **+inf** and **-inf**, can be used in places where numbers are expected. They represent plus and minus infinity.

The master file contains all instructions and options needed by all the programs of the XD package. It is created by XDINI, which provides an interface between XD and other commonly used crystallographic packages. The master file is divided into segments. Each program has its own input segment. The only segment which is shared by all the programs contains only general crystallographic information. Each line in a segment begins with a mnemonic string, usually followed by further keywords and/or numeric strings offering different sub-options or assigning default values to variables. In case of a multiple choice a sub-option can be selected by the asterisk (*) right before the corresponding keyword. Multiple flags, if not otherwise specified, are generally not allowed. Their presence should not normally terminate the program, but only the last selected option is actually activated.

A segment should begin with the module name as follows:

MODULE (*)*xdprogram*

where *xdprogram* is one of the program names (for example XDLSM, XDFOUR or XDPROP).

A new line is read until the

END *xdprogram*

card which is the normal way to terminate the program.

A special type of input section is a structured sub-segment, which can be called a *Table*. It consists of a set of lines with ordered alphanumeric fields. The first row is a heading composed of keywords showing the content of the columns. The first keyword in this row serves as *Table Identifier (TI)* the others are not interpreted (one can't use them to change the order of the fields, for example). No field can be skipped but the last one can always be omitted if a default value is available. A *Table* ends with the **END TI** instruction.

Example:

```
ATOM atom0 ax1 atom1 atom2 ax2 r/l tp tbl kap lmx sitesym chemcon
O(1) O(2) X O(1) C(1) Y R 2 1 1 4 NO
O(2) O(1) X O(2) C(2) Y R 2 1 1 4 NO O(1)
...
END ATOM
```

2.2.1 General instructions

The master file begins with a section containing basic crystallographic data, common to all programs, as follows.

2.2.1.1 TITLE

TITLE *compound-id title-string*

The first eight characters serve as a compound identifier (CID) which is used to check if certain files belong together. The CID found in the first record of `xd.hkl` and `xd.inp` files has to match with that in the master file, otherwise XDLSM terminates with an error message.

2.2.1.2 CELL

CELL *a [1] b [1] c [1] alpha [90] beta [90] gamma [90]*

Unit cell parameters are given in Å and degrees. Default angles are 90 degrees, default axis lengths 1 Å.

The additional entry **CELLSD** may also be given. It is used by XDGEOM (Chapter 5) to compute errors on derived parameters which take the cell errors into account.

CELLSD $\sigma(a)$ $\sigma(b)$ $\sigma(c)$ $\sigma(\alpha)$ $\sigma(\beta)$ $\sigma(\gamma)$ - no defaults

2.2.1.3 WAVE

WAVE *wavelength*

Radiation wavelength in Å.

2.2.1.4 LATT [C P]

LATT *centrosymmetry-flag lattice-type*

The centrosymmetry flag must be given as either **A** (non-centrosymmetric) or **C** (centrosymmetric). Lattice type may be **P**, **I**, **R**, **F**, **A**, **B**, or **C**. Rhombohedral lattices indexed on hexagonal axes (lattice type **R**) must be given as the obverse cell ($-h+k+l=3n$). Note that rhombohedral lattices indexed on rhombohedral axes have lattice type **P**.

2.2.1.5 SYMM

SYMM *general-position-coordinates*

SYMM *tx r11 r12 r13 ty r21 r22 r23 tz r31 r32 r33*

The positions may be given exactly as in the International Tables, the three coordinates being separated by commas (spaces are insignificant here). Alternatively, the operator elements may be separated by spaces (with no embedded spaces). Positions generated by a center of symmetry or corresponding to lattice centering should be omitted, and the origin must be at the center of symmetry in centrosymmetric structures. The entry 'SYMM X,Y,Z' is always assumed and will be ignored if given. More than one position may be given within one **SYMM** entry, if desired, by placing a semicolon between each of them, *e.g.* for space group $I4_1$ (no. 80):

```
LATT    A      I
```

SYMM $-X, -Y, Z; -Y, 1/2+X, 1/4+Z; Y, 1/2-X, 1/4+Z$
 or a **SYMM** entry may be given for each position.

The symmetry operation can also be written in a purely numerical way by giving a translation vector and a 3×3 rotation matrix, for example:

SYMM 0. 0. -1. 0. 0.5 1. 0. 0. .25 0. 0. 1.

Note, that a mixture of the two ways of giving a symmetry operator (SHELX-type input) is not allowed.

2.2.1.6 BANK [CR | SCM | BBB | VM]

BANK databank type

The databank type can be CR, BBB, SCM or VM (see Section 2.5 for a detailed description). In the absence of the BANK instruction, the databank CR is used as default.

2.2.1.7 INCLUDE <filename>

This instruction allows the user to include an external file containing further XD instructions. These instructions will be inserted at the point of the **INCLUDE** instruction, and **INCLUDE** instructions may be placed anywhere in the master file. An example of its use might be in XDPROP, when an extensive set of **CPSEARCH** and **BPATH** instructions are needed to calculation the topology. If all these instructions are placed in a separate file, it is only necessary to comment out a single line in the xd.mas file to remove this calculation. Include files may themselves contain **INCLUDE** instructions - there is no practical limit to the level of nesting. The allowed syntax is :

```
INCLUDE <filename>
INCLUDE "<filename>"
INCLUDE '<filename>' or even
INCLUDE<filename>
```

where <filename> is a character string, the name of the file with the XD instructions.

2.3 The parameter file xd.inp and xd.res

Type: ASCII, free-format, sequential

These are the input and output parameter files of XDLSM, and contain the information needed to calculate the electron density and related properties by XDPROP. xd.res is overwritten after each least squares cycle. See **Table 2-1** (end of this Chapter) for a detailed description.

Important! These files should not normally need to be edited.

Many entries are also present in the master file. Specifications given in the master file have the priority. It means that the xd.inp and xd.res may differ according to any changes made in xd.mas.

2.4 The reflection file xd.hkl

Type: ASCII, free-format, sequential

An input file containing the observations. It consists of as many records as observations are available. Unless anisotropic extinction is being refined, this file should normally contain only the unique reflections, with all space-group extinctions removed. If phase constraints

are to be utilised, the seventh data item must be the phase angle (in radians). See **Table 2-2** (end of this Chapter) for a detailed description.

2.5 The databank files **xd.bnk_***

Type: ASCII, free-format, sequential

These files contain ground-state STO-HF atomic wave functions for elements from H to Xe including chemically relevant ions. The basis functions are Slater type orbitals of the form:

$$b_{nl} = N_{nl} r^{(n-1)} \exp(-\zeta_n r) Y_{nl}$$

An atomic function is

$$a_{nl} = Y_{nl} \sum_k b_{knl} C_k$$

where Y_{nl} are complex spherical harmonics. The orbital coefficients C and exponents ζ are stored and used to calculate core and valence scattering factors according to a given 7electronic configuration. Additional data are also stored. A segment for an atom contains the entries given in **Table 2-3**. The files can be extended by introducing *new* segments identified by *new* atomic symbols. The element names are those conventionally used; first character upper case, second (if any) lower case. For ions the element name is followed by the order of ionization and the sign. Correct element names are: **H Na Cu2+ F-**

Important! One should not modify the values of the available entries. This can be done, if necessary, in the `xd.mas` file with the **SCAT** table entries.

The databank file `xd.bnk`, distributed in the previous versions of XD (up to Rev 1.14, 1999), is no longer valid because the introduction of new wave functions and analytical scattering factors required some changes in the format.

Four databanks are now available:

xd.bnk_RHF_CR: (flag **CR**)

Elements H-Kr: This contains the original XD databank in the new format. Clementi and Roetti [1] wave functions are tabulated for all neutral atoms and principal ions up to Kr. Single- ξ functions are taken from Clementi and Raimondi [2]. Analytical spherical scattering factor are from International Tables [3]. There are two changes with respect to the original file:

- For the metals Cr and Cu (both $4s^1 3d^5$), the 4s orbital is now included in the "core" in agreement with the default convention adopted for all other transition metals
- The analytical spherical scattering factor (SPH) is now written with 13 entries: $(a(i), b(i), (i=1, 6)), c$. Because the standard expansion of International Tables is up to $i = 4$, entries 9-12 are 0.0; the 13th entry is the constant term (which used to be the 9th entry, when only nine fields were present in the old file).

xd.bnk_RHF_BBB: (flag **BBB**)

Elements H-Xe: Wave functions are taken from non-relativistic calculations by Bunge *et. al* [4] and include all neutral atoms up to Xe. Single- ξ functions are taken from Clementi and Raimondi [2] or Clementi and Roetti [1] (for atoms of the 5th row). All the other parameters are identical to CR databank.

xd.bnk_RDF_SCM: (flag **SCM**)

Elements H-Xe (incl. Cs+): Wave functions fitted to a relativistic Dirac-Fock solution are taken from Su and Coppens [5] for neutral atoms up to Kr and from Macchi and Coppens [6] for neutral atoms Rb-Xe and all chemically relevant ions up to I-. The analytical spherical scattering factor is taken from the same publications, where a six-term fitting was used (without constant term). Single- ξ functions as for databank BBB.

xd.bnk_PBE-QZ4P-ZORA: (flag **VM**)

Elements H-Cf: STO atomic relativistic ZORA wavefunctions (Volkov & Macchi, unpublished work) obtained at PBE/QZ4P level of theory for neutral atoms H-Cf ($Z=1-98$) in the ground state configuration. The single- ξ exponents come from fitting of the density for each given orbital, and are thus slightly differ from the standard Clementi and Raimondi single- ξ functions.

All databanks now include an entry for Deuterium (D) which is identical to Hydrogen apart from the atomic weight and neutron scattering length.

Sample databank entry

```
:C      6 12.0110  0.0033  0.0016  0.0181  0.0091  6.646  77  77 185
SPH 2.3100 20.8439 1.02 10.2075 1.5886 0.5687 0.865 51.6512 0.000 0.000 0.000 0.000 0.216
SZ    5.6727  1.6083  0.0000  0.0000  1.5679  0.0000  0.0000  0.0000 0.0000 0.0000
0.0000 0.0000
STO 1s  2  6 2s -2  6 2p -2  4
      0.932620  5.435990 1  0.069310  9.482560 1  0.000830  1.057490 2 -0.001760  1.524270 2
      0.005590  2.684350 2  0.003820  4.200960 2
-0.208140  5.435990 1 -0.010710  9.482560 1  0.080990  1.057490 2  0.750450  1.524270 2
      0.335490  2.684350 2 -0.147650  4.200960 2
      0.282410  0.980730 2  0.546970  1.443610 2  0.231950  2.600510 2  0.010250  6.510030 2
```

2.6 The Fourier file xd.fou

Type: binary, sequential

A binary Fourier file is created by XDLSM, if requested, after the last least-squares cycle. It has as many records as observations were included in the structure factor calculation. An additional record at the end of the file reports the value of $F(000)$, which is needed to ensure correct scaling for Fourier maps. Each record contains the following entries:

h k l fobs sig phase amod1 bmod1 amod2 bmod2

where

h, k, l reciprocal lattice components of the scattering vector

fobs observed structure factor (normally with anomalous dispersion removed)

sig error of *fobs*

phase phase angle calculated with the final parameters according to the model the refinement was based on

amod1 real part of the calculated structure factor (*fmod1*) based on an input dependent model (MODEL1)

bmod1 imaginary part of *fmod1*

amod2 real part of *fmod2*

bmod2 imaginary part of *fmod2*

The utility programs FOU2ASC and ASC2FOU convert this binary file into ASCII format and vice-versa. This allows users to transfer the file between different computer platforms and to get a readable output for other purposes.

2.7 The design matrix **xd.der**

Type: binary, sequential
nref, *ibuf*(4), *nv*
 followed by $i=1, nref$ records of
h(*i*), *k*(*i*), *l*(*i*), (*D*(*i*,*j*), $j=1, nv$), *wt*(*i*)

D (real*8) is the matrix of derivatives of the structure factors with respect to the parameters refined (the design matrix), *nv* and *nref* are the number of variables and observations respectively, and *h*(*i*), *k*(*i*), *l*(*i*), (integer) and *wt*(*i*) (real*8) are the Miller indices and weight of the *i*'th observation.

2.8 The normal equation matrix **xd.mat**

Type: binary, sequential

nv
 (*B*(*i*,*j*), $j=1, i$), $\delta y(i), i=1, nv$
 where *B* and δy (real*8) are the coefficient matrix and vector of the system of least squares equations and *nv* is the number of variables refined:

$$B(i, j) = \sum_{h,k,l} w(h, k, l) * d|F(h, k, l)| / dp_i * d|F(h, k, l)| / dp_j$$

$$\delta y(i) = \sum_{h,k,l} w(h, k, l) * d|F(h, k, l)| / dp_i * (F_o - F_c)$$

2.9 The variance-covariance matrix **xd.cov**

Type: binary, sequential
 See **Table 2-4** (end of this Chapter) for a detailed description.

2.10 Grid and path file format

Type: ASCII, formatted, sequential
 See **Table 2-5** (end of this Chapter) for a detailed description.

2.11 XD – The Master Control Program

SYNOPSIS

xd (*options*) (*cid* (*mid*))

OPTIONS

- v** be more verbose (in XD itself, does *not* influence the output of individual modules)
- d** debug mode, show which commands would be executed, do not actually start them.
- e** <exclude-list>
modules *not* to start, although they might be flagged in the master file

- i** *<include-list>*
modules to start, whether flagged in the master file or not
- o** *<only-list>*
exclude all modules not mentioned in this list

DESCRIPTION

The modules flagged 'active' in the master file (*xd.mas*) are started. (Subject to change with the **-i**, **-e**, **-o** switches). The parameters *cid* and *mid* are passed to each module. If no master file can be found, XDINI will be started. See Chapters 9 & 10 for details about starting programs XDGRAPH and TOPXD respectively

It is also possible to start each program by its own command:

xdini *cid prgname bnkname*

See Chapter 3 for details about starting XDINI.

xdism *cid (mid)*

xdprop *cid (mid)*

xdfour *cid (mid)*

xdgeom *cid*

xdfft *cid*

xdgraph *options*

topxd *<output file>*

Bibliography

1. E. Clementi and C. Roetti. *Atomic Data and Nuclear Data Tables* **14** 177-478 (1974).
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4. C. F. Bunge, J. A. Barrientos, A. V. Bunge *At. Data Nucl. Data Tables*, **53**, 113-162 (1993).
5. Z. Su and P. Coppens *Acta Cryst.*, **A54**, 646 (1998).
6. P. Macchi and P. Coppens *Acta Cryst.*, **A57**, 656 (2001).
7. R.F. Stewart, E.R. Davidson and W.T. Simpson, *J. Chem. Phys.* **42**, 3175 (1965).

Table 2-1: The content[¶] of the parameter file. The order of the parameters (U_{ij} , C_{ijk} , D_{ijkl} , P_{lm} , $extcn$) corresponds to the list given in Table 4-2

Record	Content	Description
1	<i>xdparfile version [1/2]</i>	version of the parameter file (1 is the older, 2 the most recent one)
2	<i>cid</i>	Compound identification
3	<i>nat, ntx, lmx, nzz, nto, nsc, ntb, nov</i>	software limits for some parameters in the current program version
4	<i>(kv(i), i=1,14)</i>	Dimensions of certain arrays in XDLSM, see table 4.1 in Chapter 4 for their meanings. 1: number of atoms (<i>na</i>), 2: number of displacement tensor components (<i>ntmx</i>), 3: maximum level of multipole expansion (<i>npolmax</i>), 4: number of kappa sets (<i>nz</i>), 5: not used (<i>nto</i>), 6: scale factors (<i>ng</i>), 7: extinction model (<i>next</i>), 8: number of constraints (<i>ncon</i>), 9: number of scattering factor tables (<i>ntbl</i>), 10: number of symmetry cards (<i>ns</i>), 11: number of variables (<i>nv</i>), 12: (<i>nqq</i>), 13: number of cycles (<i>nc</i>), 14: number of dummy atoms (<i>nad</i>)
5	<i>r1o, r2o, r1, r2, r1w, r2w, gof, sig</i>	Statistics of the fit
6	<i>a, b, c, d, e, f</i>	Parameters of the lsq weight
7...+ <i>nad</i>	<i>dx(i), dy(i), dz(i)</i>	Dummy atom coordinates
do n=1, <i>na</i>		
+1	<i>atom, icor1, icor2, nax, nay1, nay2, jtf, itbl, isfz, lmax, isym, ichcon, x, y, z, amult</i>	Atom name (character*8) Code integers for defining the site coordinate system, The order of displacement tensor, scattering factor number, kappa set number, max. level of spherical harmonics used, site symmetry code (see Tables 3-1 & 3-2, Appendix), chemical constraint, fractional coordinates, multiplicity
+2	<i>U</i> for <i>jtf(n)=1</i> or <i>U_{ij}</i> for <i>jtf(n)≥2</i>	Isotropic or anisotropic <i>U</i>
+3,+4	<i>C_{ijk}</i> for <i>jtf(n)≥3</i>	3. order anharmonic tensor components
+5...+7	<i>D_{ijkl}</i> for <i>jtf(n)=4</i>	4. order anharmonic tensor components
+8...+10	<i>(Plm(j), j=1, npx)</i> <i>npx=lmax*lmax+2*lmax+2</i>	Multipole populations
end do		
+1...+ <i>nzz</i>	<i>ifz(i), (z(j,i), j=0, lmax+2)</i>	Scattering factor table to which the i'th kappa set refers, 6 kappa values
+1	<i>(extcn(i), i=1,7)</i>	Extinction parameters
+1	<i>out</i>	Overall thermal parameter
+1	<i>(sc(i), i=1, nsc)</i>	Scale factor

[¶] The previous format is still accepted and interpreted by the code

Table 2-2: The content of the reflection file.

Record	Content	Description
1	<i>cid</i> , <i>fcod</i> , NDAT <i>ndat</i>	Compound ID F or F² Number of entries for each observation (min.=6, max.=14)
do n=1,nref		
	<i>h, k, l</i> <i>iscgrp</i> , <i>obs</i> , <i>sigobs</i> , <i>tbar</i> , <i>u1,u2,u3</i> , <i>v1, v2, v3</i> <i>phase-angle</i> <i>wavel</i>	Reflection indices Scale group number <i>F</i> or <i>F²</i> as given by <i>fcod</i> <i>Sigma(F)</i> or <i>sigma(F²)</i> Absorption weighted path length (cm) Direction cosines of a vector defined with respect to the real crystal axes and normal to the plane of diffraction Direction cosines of a vector defined with respect to the real crystal axes lying in the plane of diffraction and perpendicular to the incident beam Alternatively, the seventh data item <i>tbar</i> may be replaced by the <i>phase-angle</i> (radians). This format initiates the phase-constrained refinement, and in this case NDAT must be -7 Wavelength (Å) for individual reflection in TOF data
end do		

The exact contents of the reflection file are signified by the **NDAT** parameter. The list below shows the applicable contents. The *tbar* values are necessary for the extinction correction and if absent, i.e. **NDAT** = 6, a default unitary value of 0.05 cm (or 0.5 cm for neutron data) is assumed for all reflections and a warning is issued in XDLSM. The direction cosines *u* and *v* are necessary for an anisotropic extinction correction. Note that these direction cosines follow a completely different definition from those commonly used in the SHELX programs and that they will need to be supplied by your data-reduction program (also the actual individual *tbar* values). For TOF data, the *wavel* values are also required for any extinction correction, either isotropic or anisotropic (currently only possible for neutron data).

NDAT	Contents and order of data items (free format)
6	<i>h, k, l, iscgrp, iscgrp, obs, sigobs</i>
7	<i>h, k, l, iscgrp, iscgrp, obs, sigobs, tbar</i>
-7	<i>h, k, l, iscgrp, iscgrp, obs, sigobs, phase-angle</i>
8	<i>h, k, l, iscgrp, iscgrp, obs, sigobs, tbar, wavel</i>
13	<i>h, k, l, iscgrp, iscgrp, obs, sigobs, tbar, u1,u2,u3, v1, v2, v3</i>
14	<i>h, k, l, iscgrp, iscgrp, obs, sigobs, tbar, u1,u2,u3, v1, v2, v3, wavel</i>

Table 2-4: The content of the variance-covariance file.

<i>nv, errwt</i> (real*4)	Number of variables, square of GOF
<i>((A(i,j),j=i,nv),i=1,nv)</i> (real*4)	A = <i>inv(B)</i> * <i>errwt</i> , where B is the least squares matrix
<i>(iatom(i),i=1,nv)</i>	> 0 the sequence number of the atom to which parameter <i>i</i> relates = 0 <i>i</i> is not an atomic parameter < 0 point to Kappa set
<i>(itype(i),i=1,nv)</i>	The order number of parameter <i>i</i> as described in Table 4.2
<i>(isfz(iatom(i)),i=1,nv)</i> if <i>iatom(i)>0</i>	Kappa set

Table 2-3: The content of an entry in the databank file.

Record	Rec.-Id	Entries
1.	:ELEM	<i>z w dfpmo dfppmo dfpcu dfppcu sctl ira irc irr</i> <i>elem</i> Element symbol (H, Cu, Ti3+, ...). It serves as the segment's identification <i>z</i> Atomic number <i>w</i> Atomic mass <i>dfpmo</i> Anomalous correction for Mo radiation ($\Delta f'$) <i>dfppmo</i> Anomalous correction for Mo radiation ($\Delta f''$) <i>dfpcu</i> Anomalous correction for Cu radiation ($\Delta f'$) <i>dfppcu</i> Anomalous correction for Cu radiation ($\Delta f''$) <i>sctl</i> Coherent neutron scattering length <i>ira</i> Atomic radii <i>irc</i> Covalent radii <i>irr</i> Van der Waals radii
2.	SPH	<i>a1 b1 a2 b2 a3 b3 a4 b4 a5 b5 a6 b6 c</i> Expansion coefficient for analytical approximation of the RHF spherical atomic scattering factors. For the hydrogen atom see Stewart <i>et al</i> [7]
3.	SZ	<i>(zet1(i),i=1,12)</i> <i>zet1</i> Single- ζ exponents used for the radial functions of the valence deformation density [2]
4.	STO	<i>((orb(i),ioc(i),nbf(i)),i=1,12)</i> <i>orb</i> Orbital type (1s,2s,3s,4s,2p,3p,4p,3d,4d,4f,5s,5p) <i>ioc</i> Occupation – negative number refers to valence electrons <i>nbf</i> Number of basis functions
5.		<i>((bc(i,j),bx(i,j),nr(i,j)),j=1,nbf(i),i=1,noc)</i> <i>bc</i> Coefficient of the basis function (C) <i>bx</i> Exponent of the basis function (ζ) <i>nr</i> <i>n</i> <i>noc</i> Number of occupied atomic orbitals (<i>ioc(i)≠0</i>)

Table 2-5 The content of grid and path files.

Record	Content	Description
1	<i>filetype version</i>	<i>filetype</i> can be any of 2DGRDFILE , 3DGRDFILE or PATHFILE . <i>version</i> gives the version number of the file format (currently 0).
2	<i>cid property</i>	Compound id and name of the mapped property
3	<i>title</i>	Title string
4	<i>nx ny (nz)</i>	Number of grid points
5	<i>ox oy oz</i>	Origin of the grid in 'world-coordinates'
6	<i>xdim ydim zdim</i>	Physical size of the grid (in Å)
7	<i>no</i>	Number of objects
+1...+no	<i>name x y z (type)</i>	<i>type</i> is either ATOM or CP
+1	<i>nc</i>	Number of connections
+1...+nc	<i>object1 object2</i>	List of bonds or other connecting lines to be drawn
The body for grid files		
	<i>values</i>	List of grid values, <i>x</i> varying fastest.
The body for path files		
+1	<i>ncurve</i>	Number of bond path curves
<i>ncurve</i> times		
+1	<i>object</i> <i>npoints</i>	<i>object</i> gives a starting point (usually a CP object). <i>type</i> is BOND .
+1...+npoints	<i>type</i> <i>x y z</i>	