Chapter 12

Example input files

11.1 Parameter file (XD.INP/XD.RES)

The new version of the parameter file has the following format:

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! <<< X D PARAMETER FILE >>> $Revision: 2016.01 (May 05 2016)$       27-May-16!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
XDPARFILE VERSION  2
   XD       MODEL   0  0  0  0
LIMITS nat  2000 ntx  31 lmx  4 nzz  30 nto  0 nsc  20 ntb  20 nov   2020
USAGE     17   0  0   4   0   1   0   0   4   2     0   0   0  0
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 0.000E+00
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
Fe(1)     3 2   10   1   9 2  1  1 0  0   0  0.265639  0.027046  0.283611 1.0000
  0.011940  0.012980  0.013260 -0.000650  0.005460 -0.001840
  6.0000  0.0000
.
.
.
H(32)     3 2    7  15  14 1  4  4 0  0   0  0.006430  0.094144  0.237667 1.0000
  0.036820  0.000000  0.000000  0.000000  0.000000  0.000000
  1.0000  0.0000
H(41)     3 2    8  16  17 1  4  4 0  0   0  0.107053  0.311014  0.123888 1.0000
  0.035140  0.000000  0.000000  0.000000  0.000000  0.000000
  1.0000  0.0000
H(42)     3 2    8  17  16 1  4  4 0  0   0  0.264985  0.418857  0.212776 1.0000
  0.038610  0.000000  0.000000  0.000000  0.000000  0.000000
  1.0000  0.0000
  1  1.000000  1.000000  1.000000  1.000000  1.000000  1.000000
  2  1.000000  1.000000  1.000000  1.000000  1.000000  1.000000
  3  1.000000  1.000000  1.000000  1.000000  1.000000  1.000000
  4  1.200000  1.200000  1.200000  1.200000  1.200000  1.200000
 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
 0.0000E+00
 0.132280E+01
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

The old format style is still accepted and interpreted, though the user must be aware that some default definitions have been changed (see Section 2.5 for example) and therefore parameters refined with older version of XD (and their corresponding `xd.mas` file) may no longer be consistent.

12.2 Master file

Since 2006, this is the new format of the master file. The previous format is no longer readable by XD (due to the changes in SCAT table). This is an example of a default file written by XDINI.

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! <<< X D MASTER FILE >>> $Revision: 2016.01 (May 05 2016)$          27-May-16!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
TITLE XD
CELL     11.1211    6.8670   11.1440    90.000   113.709    90.000
WAVE     0.71073
CELLSD    0.0002    0.0001    0.0002     0.000     0.001     0.000
LATT  C P
SYMM   - x, 1/2 + y, 1/2 - z
BANK CR
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
    MODULE *XDLSM
SELECT  model 0 2 1 0 based_on F test verbose 1
SELECT  cycle -1 dampk 1. cmin 0.6 cmax 1. eigcut 1.d-09 convcrit 0.0
SAVE  deriv lsqmat *cormat
SOLVE  *inv diag *cond
!-----------------------------------------------------------------------------
SCAT CORE SPHV DEFV   1S  2S  3S  4S  2P  3P  4P  3D  4D  4F  5S  5P  6S  6P  5D  7S  6D  5F  DELF'   DELF''  NSCTL
Fe   CHFW CHFW CSZD    2   2   2   2   6   6   0  -6   0   0   0   0   0   0   0   0   0   0  0.3463  0.8444  0.954
O    CHFW CHFW CSZD    2  -2   0   0  -4   0   0   0   0   0   0   0   0   0   0   0   0   0  0.0106  0.0060  0.580
C    CHFW CHFW CSZD    2  -2   0   0  -2   0   0   0   0   0   0   0   0   0   0   0   0   0  0.0033  0.0016  0.665
H    CHFW CHFW CSZD   -1   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  0.0000  0.0000 -0.374
END SCAT
!-----------------------------------------------------------------------------
ATOM     ATOM0    AX1 ATOM1    ATOM2   AX2 R/L TP TBL KAP LMX SITESYM  CHEMCON
Fe(1)    C(12)     Z  Fe(1)    C(11)    Y   R   2  1   1   4  NO
O(11)    C(11)     Z  O(11)    Fe(1)    Y   R   2  2   2   4  NO
O(12)    C(12)     Z  O(12)    Fe(1)    Y   R   2  2   2   4  NO
O(13)    C(13)     Z  O(13)    Fe(1)    Y   R   2  2   2   4  NO
C(1)     C(3)      Z  C(1)     C(2)     Y   R   2  3   3   4  NO
C(2)     H(22)     Z  C(2)     H(21)    Y   R   2  3   3   4  NO
C(3)     H(31)     Z  C(3)     H(32)    Y   R   2  3   3   4  NO
C(4)     H(42)     Z  C(4)     H(41)    Y   R   2  3   3   4  NO
C(11)    O(11)     Z  C(11)    Fe(1)    Y   R   2  3   3   4  NO
C(12)    O(12)     Z  C(12)    Fe(1)    Y   R   2  3   3   4  NO
C(13)    O(13)     Z  C(13)    Fe(1)    Y   R   2  3   3   4  NO
H(21)    C(2)      Z  H(21)    H(22)    Y   R   1  4   4   2  NO
H(22)    C(2)      Z  H(22)    H(21)    Y   R   1  4   4   2  NO
H(31)    C(3)      Z  H(31)    H(32)    Y   R   1  4   4   2  NO
H(32)    C(3)      Z  H(32)    H(31)    Y   R   1  4   4   2  NO
H(41)    C(4)      Z  H(41)    H(42)    Y   R   1  4   4   2  NO
H(42)    C(4)      Z  H(42)    H(41)    Y   R   1  4   4   2  NO
DUM0      0.0000  0.0000  0.0000
END ATOM
```

```
!------------------------------------------------------------------------------
!GROUP2   atom1 atom2 ...
KEEP     kappa  1  2  3  4
KEEP     charge group1
!KEEP     rigid group1
!RESET    bond C(1) H(1) 1.09 ...
WEIGHT   -2.0 .0 .0 .0 .0 0.3333
!SWAT g 0.00 U 0.00
SKIP     obs 0. 1.d10 *sigobs 3. 1.d06 sinthl 0. 2.
PRINT    sinthl .0 2. obs 0. 15. delta 0. 10. *del% 80 100 extcn 80. 100. *abssc
!EXTCN    *iso aniso *type_1 type_2 type_3 distr_g *distr_l msc_0  msc_1
!DMSDA    1.1  1.8
!FOUR     fmod1 4 2 0 0  fmod2 -1 2 0 0
!CON      num1 par1/iat1 num2 par2/iat2 ... = num0
!------------------------------------------------------------------------------
KEY     XYZ --U2-- ----U3---- ------U4------- M- -D- --Q-- ---O--- ----H----
Fe(1)   111 111111 0000000000 0000000000000000 00 000 00000 0000000 0000000000
O(11)   111 111111 0000000000 0000000000000000 00 000 00000 0000000 0000000000
O(12)   111 111111 0000000000 0000000000000000 00 000 00000 0000000 0000000000
O(13)   111 111111 0000000000 0000000000000000 00 000 00000 0000000 0000000000
C(1)    111 111111 0000000000 0000000000000000 00 000 00000 0000000 0000000000
C(2)    111 111111 0000000000 0000000000000000 00 000 00000 0000000 0000000000
C(3)    111 111111 0000000000 0000000000000000 00 000 00000 0000000 0000000000
C(4)    111 111111 0000000000 0000000000000000 00 000 00000 0000000 0000000000
C(11)   111 111111 0000000000 0000000000000000 00 000 00000 0000000 0000000000
C(12)   111 111111 0000000000 0000000000000000 00 000 00000 0000000 0000000000
C(13)   111 111111 0000000000 0000000000000000 00 000 00000 0000000 0000000000
H(21)   111 100000 0000000000 0000000000000000 00 000 00000 0000000 0000000000
H(22)   111 100000 0000000000 0000000000000000 00 000 00000 0000000 0000000000
H(31)   111 100000 0000000000 0000000000000000 00 000 00000 0000000 0000000000
H(32)   111 100000 0000000000 0000000000000000 00 000 00000 0000000 0000000000
H(41)   111 100000 0000000000 0000000000000000 00 000 00000 0000000 0000000000
H(42)   111 100000 0000000000 0000000000000000 00 000 00000 0000000 0000000000
KAPPA   000000
KAPPA   000000
KAPPA   000000
KAPPA   000000
EXTCN   0000000
OVTHP   0
SCALE   1
END KEY
!------------------------------------------------------------------------------
   END XDLSM
```

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
   MODULE XDFFT
SELECT   *fobs *fmod1 fmod2  snlmin 0. snlmax 2.  sig 3. phase 0.
SELECT   gridsize 0.2 scale 1. npeak 10  nhole 10  neutron  gridf  peakf
END XDFFT
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
   MODULE *XDFOUR
SELECT   *fobs *fmod1 fmod2 print snlmin 0. snlmax 2.
GRID     *3-points perp cryst
ATOM     label ato(1) symm 1 trans 0 0 0 *mark on plot
ATOM     label ato(2) symm 1 trans 0 0 0 *mark on plot
ATOM     label ato(3) symm 1 trans 0 0 0 *mark on plot
LIMITS   xmin -2.0 xmax 2.0 nx 50
LIMITS   ymin -2.0 ymax 2.0 ny 50
LIMITS   zmin  0.0 zmax 0.0 nz  1
   END XDFOUR
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
   MODULE XDPROP
!
!-----General section-----
!
SIZE     napl 8
MODEL    iam *multipole
! *au will print results in a.u. but input is always given in Ang
SELECT   numdx  esd  au  verbose 1
PROPERTY *rho gradrho d2rho defden valence core nucpot ef efg
PROPERTY  esp oep nci dori sedd ked ped ted srho eig2
!
! Define the cluster of atoms to be included:
!CRYSTAL alim [amin] [amax] blim [bmin] [bmax] clim [cmin] [cmax]
!APPLY    symm 1 translations 0 0 0 ato(1) ato(2) ...
!GROUP    ato(1) ato(2) ... (atom label)
!OMIT     1 2 ... 4 -8 (number in atom list)
!
! Parameters for topological analysis:
SELECT   cpcut 1.0d-6 lmax 4  nstep 20  rcut 4.0
SELECT   scale 0.05  dx 0.001  ds 0.005 dncut 0.0
SELECT   rEcrit 0.00001  rNcrit 0.00001
SELECT   dncut 0.0 rhocut1 0.0 rhocut2 0.0
!
! Parameters for the integration routine:
ODESOLVE *rk bs eps 1.D-06 stepi 0.01
QUADINT  iqt 2  Nrad 50  Nang 194  Becke  *Stock
!
```

```
! Method for calculation of ESP/EF/EFG
EPFG  EP aMM mMM *EPMM  rCrit1 6.0 rCrit2 15.
! Origin of the coordinate system for molecular moments
ORIGIN  *mass charge geom ucell
!
! Export atomic moments to Orient/MIN16
!EXPORT  *orient *min16 lmax [4] nmol [k] natmol [i=1..k]
!
!------End of General section-----
!
! Atomic/Molecular moments from pseudoatoms :
MULTMOM
!
! Calculate d-orbital populations for transition metals
!D-POP use *Pv *P00
!
! Atomic/Molecular from STOCKHOLDER partitioning:
!STOCKMOM atoms all *unique select ato(1) ato(2) ...
!
! Evaluation of intermolecular interaction energy and lattice energy:
!
!ATATPOT  *EXREP spack  *wilcox lj
!ATATPOT  *DISPR spack  *wilcox lj
!HBONDS   atoH(1) ato(1) rHBOND(1) atoH(2) ato(2) rHBOND(2) ...
!HPOLAR   atoH(1) atoH(2) ....
!
!INTEREN  frag 1  nat1 -nat2 *neutral
!INTEREN  frag 2  nat3 -nat4 *neutral
!INTEREN  EP aMM  mMM *EPMM  rCrit1 4. rCrit2 15.
!
!LATEN    frag1 1 -10  *neutral
!LATEN    radii  0. 100.
!LATEN    EP aMM  mMM *EPMM  rCrit1 4. rCrit2 15.
!
NUCPROP (*)all (*)selected [n1] [n2] [-n3] ...
!
! Atomic charges fitting electrostatic potential:
!QFIT     grid 11 length 7.0 width 1.0 constrain false
!CONSTRAIN ato(1) ato(2) ...
!
! Function plots:
!POINT    x y z
!LINE     ato(1) ato(2)  npts 50
!LINE     points x1 y1 z1 x2 y2 z2 npts 50
```

```
!VECPLOT  *labels *zcut 1.2 omitrad 0.2 *vcut 0.8  vscale 1. xytol 0.4
!MAP      atoms ato(1) ato(2) ato(3) npts 50 stepsize 0.1
!MAP      bvect1 x1 y1 z1 bvect2 x2 y2 z2 cen x0 y0 z0 npts 50 stepsize 0.1
!CUBE     centre x y z   npts 30  stepsize 0.1
!CUBE     ato(1) ato(2)  npts 20  stepsize 0.1
!CUBE     hirshf xd_iam_mol.grd xd_iam_cry.grd
!
! Gradient field plots (only for rho and esp functions):
!TRAJPLT  origin atom ato(1)
!TRAJPLT  xaxis  atom ato(2) Xdim1 -3.0 Xdim2 3.0
!TRAJPLT  yaxis  point x y z Ydim1 -3.0 Ydim2 3.0
!TRAJPLT  mark *atoms *labels *bonds *cps *basins *hbonds
!TRAJPLT  params Circle 0.1 ATrad 0.05 CPrad 0.08 CPgrid 0.3 CPlim 1.0d-4
!TRAJPLT  *plot *plane npath 36 *zcut 0.3 *xytol 0.5 *all select ato(1)
!
! Local Source Function (only for rho and esp functions):
!SOURCE   refpoint x y z
!SOURCE   point x y z
!SOURCE   line  ato(1) ato(2)  npts 50
!SOURCE   map atoms ato(1) ato(2) ato(3) npts 100 stepsize 0.1
!SOURCE   cube ato(1) ato(2) ato(3) npts 20 stepsize 0.1
!
! Topological analysis:
!CPSEARCH bond ato(1) ato(2)
!CPSEARCH bond rmin  1.2 rmax  1.6
!CPSEARCH ring ato(1) ato(2) ...
!CPSEARCH shell ato(1) rmin 0.3 rmax 0.5 nrad 5 nang 11 11 cutoff 16.0
!CPSEARCH bubble ato(1) rmin 0.3 rmax 0.5 curv -3 ncps 3
!CPSEARCH point x y z
!CPSEARCH line vec1 x1 y1 z1  vec2 x2 y2 z2  npts 15
!CPSEARCH start file.cps
!BPATH    ato(1) ato(2) algrithm 2
!MOLGR    *auto level 1 rmin 0.8 rmax 3.5  algrithm 2  profile
!
! Atomic basin integration:
!TOPINT step 0.01 accur 0.001 rmax 8.0 nmax 20
!TOPINT spheres ato(1) r1 ato(2) r2 .....
!TOPINT atoms all *unique select ato(1) ato(2) ...
!
   END XDPROP
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
   MODULE XDGEOM
SELECT   rmin 0.8 rmax 1.8  tor *ato *bon *ang loc non *export
   END  XDGEOM
```

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
   MODULE XDVIB
SELECT   temp 100. scale 1. *nlinear linear
MODES    *all frqmin 0. frqmax 1500.
!MODES    include 1 2 3 ...
!MODES    exclude 1 2 3 ...
DATAFILE *gaussian g98.out orient *standard input
   END  XDVIB
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
   MODULE TOPXD
SIZE napl 2000
COMT just a comment for this run
DEBG symeqv deriv check
TRSH eigenvec 1.0d-10 nr 1.D-08
CGEN alim -0.5 1.5 blim -0.5 1.5  clim -0.5 1.5
MPAR  rcut 4.0d0  dstep 5.d-3  au iam esp
!DGRD *use *gen fra gstep 0.2 0.2 0.2 read *ascii fort.69
!
!TRHO *seed all ail debug nstep 12 nnb 15 rmax 3.0 th 2.7
!  fra  0. 0. 0.
!  car  0. 0. 0.
!TRHO *cluster all ail debug nstep 11 nnb 10 rmax 3.0 th 2.7
!TRHO *pairs nr ail debug nstep 11 nnb 9 rmax 5. th 2.2 pc 0.3
!TRHO *points nr ail debug nstep 20 nnb 9 rmax 5 fra
!  0.0  0.0  0.0
!  0.5  0.5  0.5
!TRHO *line nr ail debug nstep 10 nnb 20 rmx 5. pc 0.3
!  point fra  0. 0. 0.   0.5 0.5 0.5
!  point car  0. 0. 0.    2. 2. 2.
!TRHO *grid nr ail debug nstep 10 nnb 9 rmax 5 ncons 0
!  xmin 0.  xmax 1.  xstep  0.01
!  ymin 0.  ymax 1.  ystep  0.01
!  zmin 0.  zmax 1.  zstep  0.01
!TRHO *profile perstep 2.
!  *atom ato(1) toneighbor 1 2 3
!  *point fra  0. 0. 0.   1. 1. 1.
!  *point car  0. 0. 0.   2. 2. 2.
!
!TLAP *auto ef CCCP ail debug nstep 15 nnb 10 rmax 3.0 ntheta 8 nphi 16
!  atoms ato(1) ato(2) ... nmax 0 rstar 0.d0
!  atoms ato(3) ato(4) ... nmax 2 rstar 0.d0
!  nna x 1.  y 1.  z 1.  nmax 4 rstar 3.2
!  nna x 2.  y 2.  z 2.  nmax 4 rstar 3.2
!TLAP *auto nr ail debug nstep 20 nnb 12 rmax 3.0 ntheta 16  nphi 8
```

```
!  atoms ato(1) ato(2) ... nmax 0 rstar 0.d0
!TLAP *points nr ail debug nstep 23 nnb 11 rmax 4.0 nmax 14
!  car  1. 1. 1.
!  fra  0. 0. 0.
!TLAP *line nr ail debug nstep 12 nnb 12 rmax 3.0 nmax 0
!  atom ato(1) toneighbor 1 2 3
!  points fra 0. 0. 0.  1. 1. 1.
!  points car 0. 0. 0.  2. 2. 2.
!
!ATBP Params PhInSph 48 ThInSp 32  *SavSurf
!ATBP Spheres ato(1) 0.2 ato(2) 0.2 ...
!ATBP AltGuess BigStep 0.5 Accur 0.002 MaxRInt 10.00 Rmax 10.0 Step0 0.025 A 0.0 B 0.0
!ATBP *atoms ato(1) iZFS nvi 100 IRsur 0 *IRSav Rest Debug Phi 32 Th 24 Rad 120 Accur 1.D-3
!ATBP nna 0
! x 0. y 0. z 0. *integ sphere 0.2 iZFS nvi 5 irsur -1 irsav rest debug phi 8 th 4 rad 120 ncp 0
!
!VZ3D *plot
!  files rays.dat
!  basins ato(1) ato(2) ...
!  range *default xmi 0. ymi 0. zmi 0. xma 1. yma 1. zma 1.
!  grid *default dx 0.05 dy 0.05 dz 0.05 rvec *default 0.20
!END VZ3D
!
!PL2D general
!  point car 0. 0. 0.
!  atom  1   0 -1  0
!  atom  2  -1  0 -1
!  plotdim xmin -2. xmax 2.  xstep 0.5 ymin -2. ymax 2.  ystep 0.5
!  origin ishift 5  origin 0. 0. 0. vmod 0.5
!  misc size a4 scale 0.4 name 'test2d' title 'TOPXD rulez!'
!PL2D *rhoo nstar 10 rmax 3.0 test cut 0.5  0.2
!PL2D *lapp nstar 10 rmax 3.0 test cut 0.5  0.2
!PL2D *lapm nstar 10 rmax 3.0 test cut 0.5  0.2
!PL2D *grho nstar 10 rmax 3.0 test cut 0.5  0.2
!PL2D *trajgrad nstar 10 rmax 5.0 test cut 0.5 0.2  toler 0.5 0.5 *plane npath 36 nextr 0
!PL2D *molgraph nstar 10 rmax 5.0 test cut 0.5 0.2  toler 0.5 0.5 *plane thr 1.6 *tr1 *tr2 *tr3
!PL2D *trajmolg nstar 10 rmax 5.0 test cut 0.5 0.2  toler 0.5 0.5 *plane thr 1.6 *tr1 *tr2 *tr3 npath 36 nextr 0
!
!PL3D general fra
! xmin 0.0  xmax 0.5  xstep 0.05
! ymin 0.0  ymax 0.5  ystep 0.05
! zmin 0.0  zmax 0.5  zstep 0.05
! name 'test3d'
!PL3D *plot rhoo lapp grho
```

```
!
!P2DCRY *diff rhoo file1 file2
!P2DCRY *diff lapm file3 file4
!P2DCRY  diff test2d rhoo
!P2DCRY  diff test2d trajmolg
!
   END  TOPXD
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
   MODULE XDPDF
SELECT   atom atom(1) scale 1.0 orth
CUMORD   second  third  fourth
GRID     3-points *cryst
!ATOM     label atom(2) symm 1 trans 0 0 0
!ATOM     xyz  0. 0. 0.
LIMITS   xmin -0.8  xmax 0.8  nx 51
LIMITS   ymin -0.8  ymax 0.8  ny 51
LIMITS   zmin -0.8  zmax 0.8  nz 51
   END  XDPDF
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
   MODULE XDHKL
SELECT   *merge  zero  remove  crypher
SELECT   export  stlmin 0.0 stlmax 1.1 nbatch -1
INPUT    xd.hkl
   END  XDHKL
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
   MODULE XDSFR
SELECT  *resol  hklim  hklist  print 100  Uiso 0.0
SELECT  title <title string>
UCELL   30.0 30.0 30.0 90.0 90.0 90.0
WFNFL   file <wfn filename>
INT3D   iqt  1  Nr 70  Nang 590
RESOL   stlmin  0  stlmax 1.1
HKLIM   hmin -10  hmax 10  kmin -10  kmax 10  lmin -10  lmax 10
HKLIST  file <hkl listfile>  maxref -1
EXPORT  *xd  *shelx  crystal  nbatch -1
   END  XDSFR
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

Chapter 13

XD2016 Installation

The XD2016 package is supplied as precompiled executables, for a variety of modern platforms. Once a user has registered for the package, he/she will be issued with the password(s) required to download the package from the XD website.

http://www.chem.gla.ac.uk/~louis/xd-home/

13.1 Installing XD2016 for Linux/Mac

Statically linked executables of the XD2016 package for Linux are provided for 32 and 64-bit Linux operating systems. They should run under any (relevant) flavour of Linux. The plotting program XDGRAPH is quite platform dependent, so that precompiled executables may not work properly. For this reason the source code and makefile are also supplied. To compile XDGRAPH you need an ANSI C compiler. Note that some C compilers provided as part of the operating system are *not* ANSI compatible. In addition, the ***Tcl/Tk*** libraries (available from http://www.tcl.tk) and optionally the ***OpenGL*** libraries (or substitutes such as the ***MESA*** libraries usually supplied with Linux installations) are required. The program is tested with ***Tcl/Tk*** version 8.3. The file `mk.config` will need to be edited to suit your local installation of Linux.

The program is provided in a tar GZipped archive. This should be copied to a suitable directory (probably root privileges are required) and unzipped,

```
gunzip xd2016.tar.gz
tar -xvf xd2016.tar
```

The resultant directory structure is something like :

xd2016	containing the Makefile and config files for XDGRAPH
xd2016/ports	config files for various compilers for XDGRAPH
xd2016/bin	containing all the executables
xd2016/xdgraph/src	containing the source code for XDGRAPH
xd2016/lib/xd	containing system files and databanks
xd2016/lib/xdgraph	containing system files for XDGRAPH

The environment variable XD_DATADIR points to the full pathname of xd2016/lib/xd, and the executables directory xd2016/bin need to be added to the PATH environment variable of each user. The environment variable XD_TCLDIR points to directory containing the XDGRAPH Tcl scripts,

For Mac users, dynamically linked OS-X 10 executables for the PowerPC and Intel processors are provided. These executables are linked to Mac system libraries (which should be present in all OS-X 10 environments), and also to the **gfortran** libraries. These latter libraries (and libraries for XDGRAPH) are provided in the download, and are placed in the same directory as the program executables. The environment variable DYLD_LIBRARY_PATH is essential, and points to this directory. So, for example, if you have installed XD2016 into /usr/xd2016_macm, then

```
export DYLD_LIBRARY_PATH=/usr/xd201_macm/bin:$DYLD_LIBRARY_PATH
```

13.2 Installing XD2016 for *Windows™*

XD2016 is available for *MS Windows* (XP/Vista/7/8/10 – 32- or 64-bit versions). The installation is self-contained, and includes all executables, all required run-time libraries and all system files, with no dependencies on third-part libraries. It is **strongly suggested** to install into the default directory given by the installation program. In addition, the working directory containing the XD data files (`xd.mas, xd.inp` *etc*) **should not** contain an embedded blank in its name, or all programs may not work.

Two versions (as both 32-bit and 64-bit executables) are provided :

The **console version** works like a DOS program, driven by the command line, in a virtually identical manner to the Linux/Mac versions of the program. It is necessary to open a DOS/Command prompt window, change to the working directory using "cd" and issue text commands.

The **GUI version** is controlled by the *WinXD* GUI (which has its own separate manual). The XD system programs (XDLSM, XDPROP *etc*) have exactly the same functionality as their console versions, but the text output is directed to the text window of the GUI. Programs may be executed, and the parameter and master files edited, using standard *Windows™* drop-down menus and dialog boxes. In addition to the standard functionality of XD, the *WinXD* GUI has a number of extra useful graphical features.

13.2.1 Environment variables

In order for both *Windows™* versions to function, the following environment variables need to be set

XD_DATADIR	(points to directory containing the data bank files)
XD_TCLDIR	(points to directory containing the XDGRAPH Tcl scripts)
TCL_LIBRARY	(points to directory containing the TCL 8.3 system scripts)

Example values for these variables would be

XD_DATADIR=<*xddir*>/*lib/xd*
XD_TCLDIR=<*xddir*>/*lib/xdgraph*
TCL_LIBRARY=<*xddir*>*bin**tcl8.3*\

where <*xddir*> is the fullpath of the XD installation directory, *e.g.* "c:\xd2016".

NOTE : the use of Unix style forward slashes "/" rather than DOS backslashes "\" as delimiters for the directory names with XD_DATADIR & XD_TCLDIR is essential. This is a result of porting a Unix program to Windows and is necessary for XDGRAPH to work correctly. The standard DOS backslash "\" should be used for the TCL_LIBRARY environment variable.

Finally, the console version requires that the directory <*xddir*>/*bin* is in the PATH, so that *Windows™* has access to all the executables.

13.3 External programs for XD2016

XD2016 writes a number of files (primarily graphical files) which require external, publically available programs to view. To access all the new features of XD2016, it is recommended that these programs are also installed. They are all available either as *Windows™* or Linux executables.

MoleCoolQT - a program for visualising iso-surfaces and mapped iso-surfaces

http://www.molecoolqt.de/

An excellent program written by Christian B. Hübschle is now freely available for academic users. This produces iso-surface plots directly from the XD grid files or Gaussian format cube files output by XDPROP, and alleviates the deficiencies of the *Windows™* version of XDGRAPH.

Molekel version 4.3 - a program for visualising iso-surfaces and mapped iso-surfaces

http://molekel.software.informer.com/5.4/

This program reads the Gaussian style cube files written by XDPROP. It is important to use version 4.3, rather than more recent versions (5.1 or later), since the latter do not (as yet) allow plotting of mapped isosurfaces.

Ghostview - a program for visualising PostScript files

http://www.ghostscript.com/download/

This program reads the PostScript files written by XDPROP.

POV-Ray - a ray-tracing program for high quality graphical rendering

http://www.povray.org/

This program reads the scene description files written by the WinXD GUI and the utility program rays2pov.

Plotmtv - a graphics program for drawing vector plots

http://rpmfind.net/linux/rpm2html/search.php?query=plotmtv

This program reads the MTVDAT files written by XDPROP and plots vector plots (as well as many other types actually). Linux rpm distributions and source code from this site.