Modifications in version 2024.1a (23 December 2024)

Modifications in XDINI

(a) the default key mask for H atoms on special positions has been modified.

Modifications in XDLSM

(a) the program now prints a warning message and halts if CHEMCON constraints between atoms with differing site occupancies are detected. Previous versions inadvertently allowed this situation but incorrectly applied the parameter shifts so that the multipoles were not actually chemical equivalent.

(b) the overall charge on the ASU is no longer printed if the scattering model code is less than -1, i.e. for conventional spherical atom, core or neutron refinements, as it is not a meaningful number.

(c) the “electroneutrality” constraint referred to in the manual and listing output of XDLSM has been renamed the “monopole population” constraint, since this is a more accurate reflection of its action.

(d) some minor I/O format changes.

Modifications in XDHKL

(a) now recognises xd.fco as an “fcf” format file

(b) now writes out xd.inp.merged & xd.mas.merged as well as xd.hkl.merged where merging was requested, these files being suitable for continued refinement of the merged hkl file (they only have one scale factor).

Bug fixes (all in XDLSM)

(i) bug in routine reading xd.mas so it nows read past 80 characters

(ii) bug in parsing the site-symmetry & CHEMCON symbols in the ATOM table of xd.mas

(iii) bug in the routine checking for unrefined parameters in CON instructions

(iv) bug in XDLSM in printing out the parameters with largest shift/su

Modifications in version 2024.1

1. Module XDINI is substantially modified and now consists of three modules:

(a) XDINI(OLD) the essentially unmodified XDINI which creates the basic XD system files

(b) XDLSDB which assigns a local symmetry and appropriate new local coordinate system and (optionally) applies the assigned local symmetry to the multipole key table. It also extends recognised X-H distances to their standard neutron-determined values and generates the

appropriate RESET BOND constaints in the master file and a set of refinement constaints in the *include* file “riding.con”

(c) XDSPOS which determines the site symmetry of atoms in special positions, assigns a new appropriate local coordination system and determines the restrictions on all refinable parameters.

(d) If CIF input is selected, XDINI runs a syntax checking program prior to running XDINI, which gives a detailed breakdown of all syntax errors. If syntax errors are found the program halts. This is because the routines which XD uses to read CIF files have problems with CIFs containing syntax errors and give enigmatic and difficult to interpret error messages.

(e) After execution of XDINI, the program prints a resume of all program comments and warnings, so that users can easily see if everything went OK.

(f) XDINI checks whether the input data files contain disordered or partially occupied atoms and gives a WARNING. All 3 modules can perform some checks on disordered atoms and the results are combined in the final warning. XDINI checks (for CIF input only) whether some atoms have occupation factors less then 1.0. XDLSDB also checks for disordered atoms, but cannot tell whether an atom in a special position is also disordered. XDSPOS checks whether atoms in special positions are disordered or partially occupied.

(g) XDINI in CIF input mode can read multipole parameters if present in the CIF and this possibility is retained. However, these populations are overwritten by XDLSDB to default values, which makes sense as the local coordinate system is changed.

(h) XDINI checks for duplicate names in resultant XD files. This can happen with both SHELX and CIF input with perfectly legal names. At present just a WARNING is issued and no action taken.

(i) XDINI checks the resolution of the data in sin(theta)/lambda and issues COMMENTS/WARNINGS as to the suitability of the data for charge density refinement.

(j) XDINI determines the space group (for CIF & SHELX input) and checks whether it involves polar axes. If necessary, it automatically applies the necessary constraints to the xyz parameters of the first atom in the list (normally assumed to be the heaviest atomic type) to fix the origin.

(k) XDINI checks whether the wavelength is non-standard (i.e. not Cu or Mo Ka) and calculates fp & fpp for all atomic species for non-standard wavelengths. These values are stored in the XD.MAS file. This program requires an external file Xsect_n.dat which is stored in the same location as the databank files.

(l) The neutron scattering length written to the XD.MAS file is now in units of Fermi’s (10^{-15}m) rather than as previously in units of 10^{-14}m, i.e. the same as stored in the databanks.

IMPORTANT: The default key mask written by the new XDINI indicates which parameters are *allowed* to be refined, not necessarily those which *should* be refined. Control of which parameters are refined is best accomplished by using the global limits or individual limits in the ATOM table. Especially for atoms in special positions, it is recommended that these should not be modified. As a consequence of these changes, the site-symmetry code (*isym*) written to the parameter file is now used to indicate the crystallographic site symmetry (codes 1-78) or the pseudo-symmetry (codes 80-

112). In previous versions this code was unused and always set to “1” in the parameter file and indicated as “NO” in the master file.

2. The calculation of the overall charge on the asymmetric unit reported by XDLSM has been modified. The calculated number of valence electrons for each element is now determined from its Z value as given in the databank minus the number of core electrons defined in the SCAT table for that element. In previous versions, the calculated number of valence electrons for each element was simply taken as the number defined as valence in the SCAT table. The calculated number of valence electrons for the ASU is the sum per atom (weighted by the atomic occupancy) and the overall charge is the difference between this number and the summed monopole populations. For experimental data, the charge on the ASU should invariably be exactly zero.

3. XDLSM now ignores CON instructions which refer to unrefined atomic parameters and issues a message. In previous versions, the program halted in this situation. The program will still halt if a CON instruction refers to unrefined non-atomic parameters (kappas, extinction parameters, scale factors).

4. The number of allowed scale factors has been increased to 99