

1.2 The UXD format

The UXD format is "universal" in the sense that it you can import easily almost any ASCII data file for XRD:

- (d, I) files (DIF patterns, peak list) or scan files of any kind, in almost any format, measured with any radiation;
- single range or multirange files.

As the data in the X-ray diffraction field are simply collections of numbers 2θ , d or I , the structure of the UXD files is very simple; it consists in two parts (for a more precise description, see Chapter 5 "The Exchange file format (UXD)"):

1. a header, containing the useful values to exploit the spectrum (such as the wavelength, step size, step time, starting angle...); these values are defined by keywords beginning by an underscore character, e.g. `_STEPTIME=2;`
2. a collection of numbers, which can be simply the intensities (for a constant step, the angles can be calculated with the starting angle and the step size) or angles followed by intensities.

There are of course restrictions to the "universality" of the UXD format. For example, the line terminator must be the carriage return/line feed combination, that is the unique line terminator used in the PC world, so you should care about that restriction when importing ASCII files from other platforms than PC. Most other restrictions are easily worked around. For instance, a fixed data collection time is assumed, but using Cps (counts per second) as input, instead of counts, can solve the problem.

Examples of how to import ASCII files in some popular formats are given in chapter 4, "Conversion Examples" of this guide. The way to export our binary files, especially to spreadsheet programs (such as Microsoft Excel), is also demonstrated in the same chapter. This will show that, despite the huge flexibility of XCH and FILE EXCHANGE (there are more than 100 keywords available), you do not need to know any of them to import data to DIFFRAC^{plus} for the most usual cases. Only a minimum of keywords, typically less than 10, has to be remembered for specific cases (exporting data never requires any remembering at all).