Chapter 2.6

XDISP

A program to calculate frequency dependent X-ray scattering factors

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The program XDISP calculates the frequency dependent components of the elemental X-ray scattering factors - the real and imaginary dispersion terms ($f´$and $f´´$) and the photon interaction cross-section (μ in barns/atom). These are necessary for refinements using SHELXL when X-radiation wavelengths other than Mo, Cu or Ag (*e.g.* from synchrotron sources) was used for data collection.

XDISP contains two computer codes which calculate $f´$, $f´´$ and μ : the original FPRIME code of Don T. Cromer [1] and the code of Sean Brennan [2] (which is derived from FPRIME). Both codes use the same dipole-approximation method of Cromer and Liberman [3], but may use slightly different X-ray cross-section data, and may give somewhat different numbers. Usually $f´$ and $f´´$ are very similar (generally much less than 1% different), but μ may differ by several percent. The Z-dependent, energy independent correction of Kissel & Pratt [4] for the relativistic real anomalous scattering factor $f´$ is used in both codes, and the Jensen term [5] (shown to be erroneous by Kissel & Pratt) is ignored in both codes.

The following Periodic Table Window opens when this menu item is selected;

The user should select the wavelength (Å) and then the chemical elements in the structure under consideration by clicking on the relevant element boxes for each element. The interpolation order is used only for the FPRIME method. Allowed values are 0-3. If the value is zero, then interpolation is by fitting three closest points to a quadratic. If other values are given, Aitkins interpolation method is used. It is usually left at the default value of 2. The calculated values of f', f'' and μ for the element at the selected X-ray wavelength are displayed in the status bar.

Using the *File-Write Element Table* menu item, the entire set of f', f'' and μ values at the chosen wavelength for every element are written to the files *table_FPRIME.lst* or *table_BRENNAN.lst* (depending on the chosen code). Using the *File-Write SHELX DISP file* menu item, the user can write SHELX format dispersion cards to the file *disp.out*. These should be pasted in the model .INS file immediately *after* the SFAC card and *before* the UNIT card. Since all the other scattering factor terms are independent of the radiation wavelength, it is only necessary to include these DISP cards as well as the normal SFAC card. This procedure is carried out automatically by *Initialise Files* if WinGX detects an unusual wavelength, (i.e. not MoKalpha, CuKalpha or AgKalpha). For example,

```
SFAC   C H O N Fe
DISP   C    0.00313    0.00161       6.46
DISP   H    0.00000    0.00000       0.67
DISP   O   -0.00411    0.00610      32.04
DISP   N   -0.00305    0.00332      19.39
DISP   Fe   0.21727    0.84965    3472.03
UNIT   24 32 4 4 2
```

The variation of f' and f'' with X-ray wavelength may be plotted over an arbitary range (limits 0.01 - 100 Å) by using the *File-Plot Dispersion Curve* menu item. If an element has been selected, the following Window opens
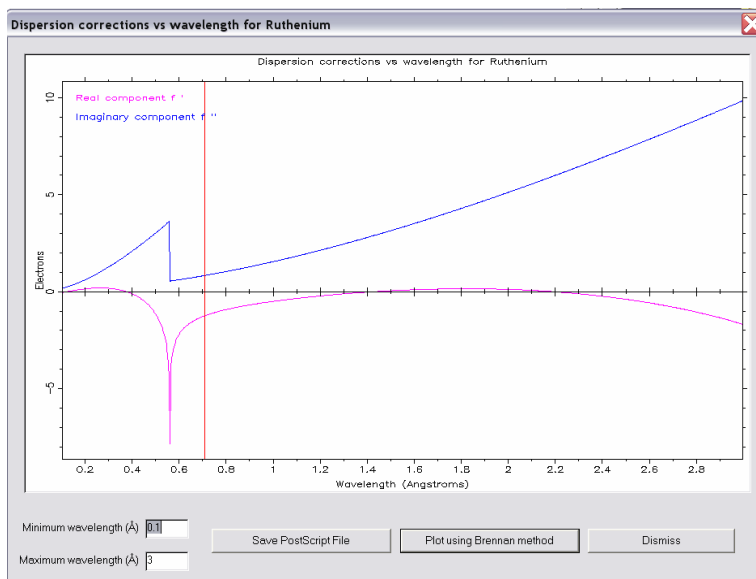
This plot can be saved as a PostScript file called *<element>_disp.ps* and the computed values of *ƒ´, ƒ˝* and µ at each wavelength increment are written to an ASCII output file *<element>_disp.out*. The Gaussian integration may fail if an X-ray energy is very close to one of the energies used, and an incorrect anomalous scattering factor *ƒ´* may result (usually very obvious in the plots). There is no easy way out of this problem. A suggested way is to compute several values at nearby energies and draw a smooth curve. This method should work, provided the points do not pass through an edge. The computed values of *ƒ´* close to an absorption edge should be regarded with particular suspicion.

References.

1.   D. T. Cromer (1983) *J. Appl. Cryst*. **16**, 437
2.   S. Brennan & P. L. Cowan (1992) *Rev. Sci. Instrum*. **63**, 850
3.   D. T. Cromer & D. Liberman (1981) *Acta Cryst* **A37**, 267.
4.   L. Kissel and R. H. Pratt (1990) *Acta Cryst* **A46**, 170.
5.   M. S. Jensen (1979) *Phys. Lett*. **74A**, 41.