

Chapter 9.12

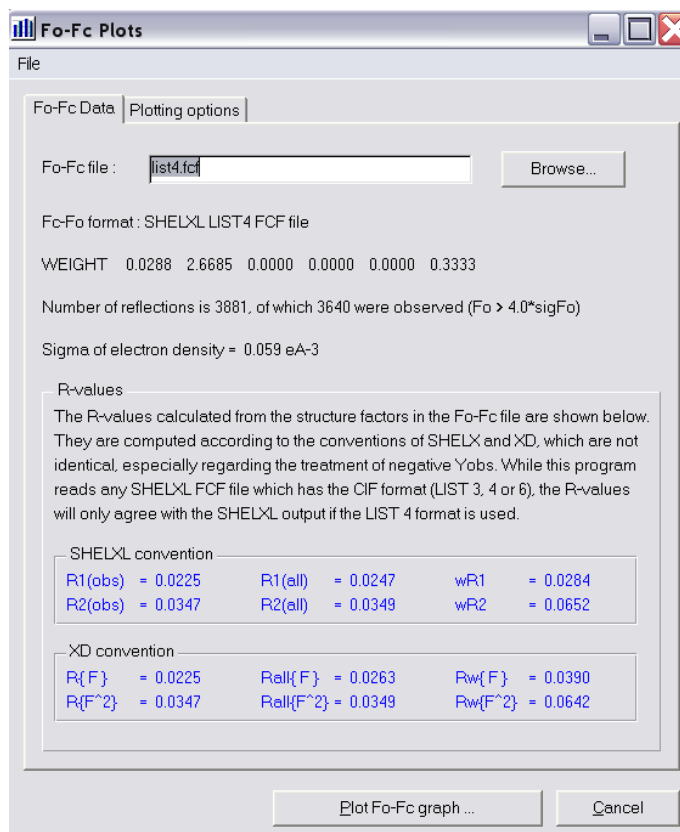
Data Plotting

Fo-Fc Plots and DRK-Plot

Louis J. Farrugia
Dept. of Chemistry
University of Glasgow
G4 9DS, Scotland, U.K.
email: louis@chem.gla.ac.uk

The **Fo-Fc Plots** program reads a CIF format structure factor file, *i.e.* *name.FCF*, written by SHELXL (either LIST 3, LIST4 or LIST 6 format, though LIST 4 format is preferred) or *XD.FCO* written by XD, and plots the resultant data in a number of ways. The DPLOT plotting program is used to visualise the graphs.

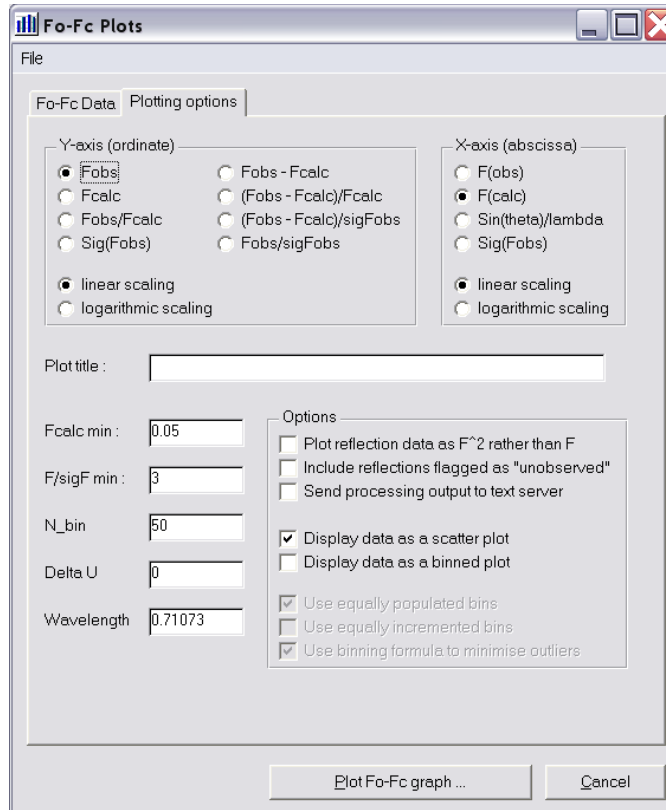
DPLOT (by David Hyde) is a very versatile plotting program, and is available for a small fee (for the fully functional version) from <http://www.dplot.com/>, or as a free cut-down version for just viewing the graphs from http://www.dplot.com/dplotviewer_setup.exe



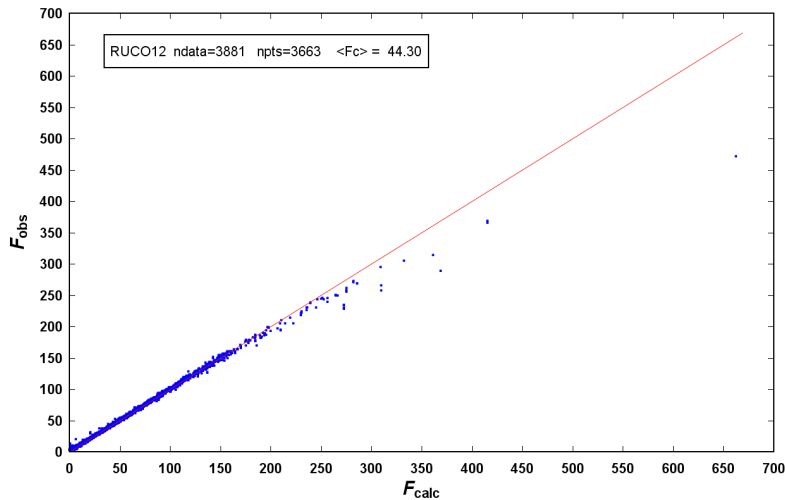
A number of standard *R* values are computed, according to the conventions of data treatment in SHELXL and XD. As well as reading the FCF file, the program attempts to obtain further information from a *name.INS* file (if SHELXL FCF file is input) or from *XD.MAS* if an *XD.FCO* file is loaded, regarding the actual weighting scheme used. The LIST 4 format (or *XD.FCO* format) is the recommended one, and the derived *R* values should agree very well with those listed in the refinement output.

The main purpose of **Fo-Fc Plots** is to obtain plots, as scatter plots or binned plots of the data, in DPLOT format. The exact data which are used for the ordinate and abscissa axes is determined by the user, using the "plotting options" pane in Control Panel, shown below.

Useful plots could be F_{obs} vs F_{calc} to show up the presence of extinction effects, or of F_{obs} vs $\sin\theta/\lambda$ to determine whether the scale factor is linear across the resolution ranges

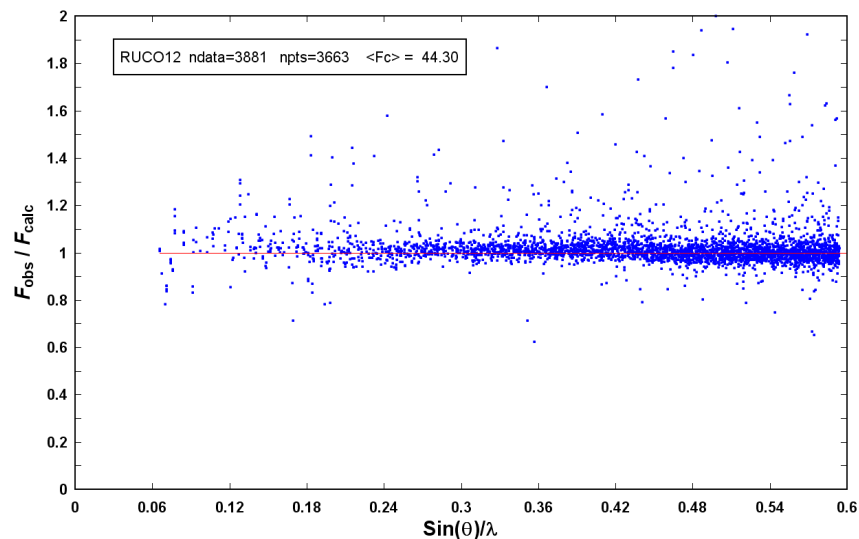


Sample plots are :

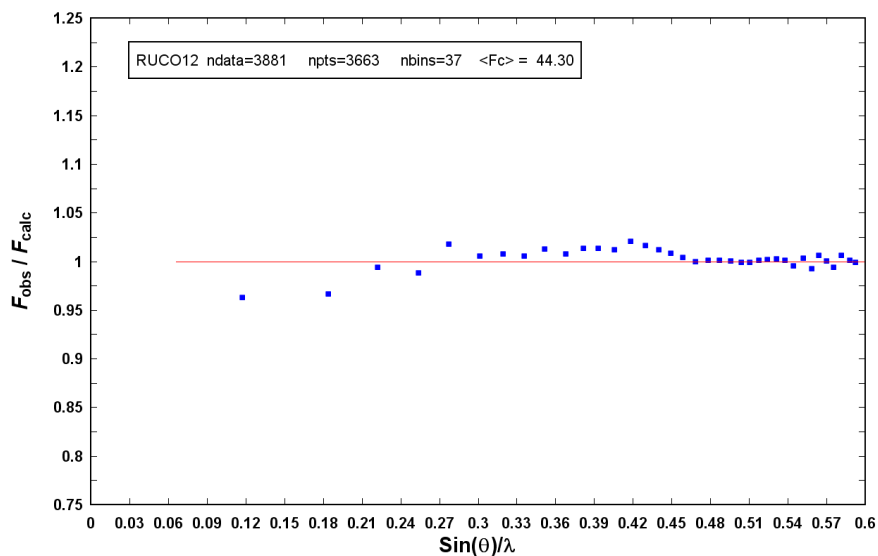


This plot clearly shows that the most intense reflections are consistently underestimated, which is indicative of extinction effects

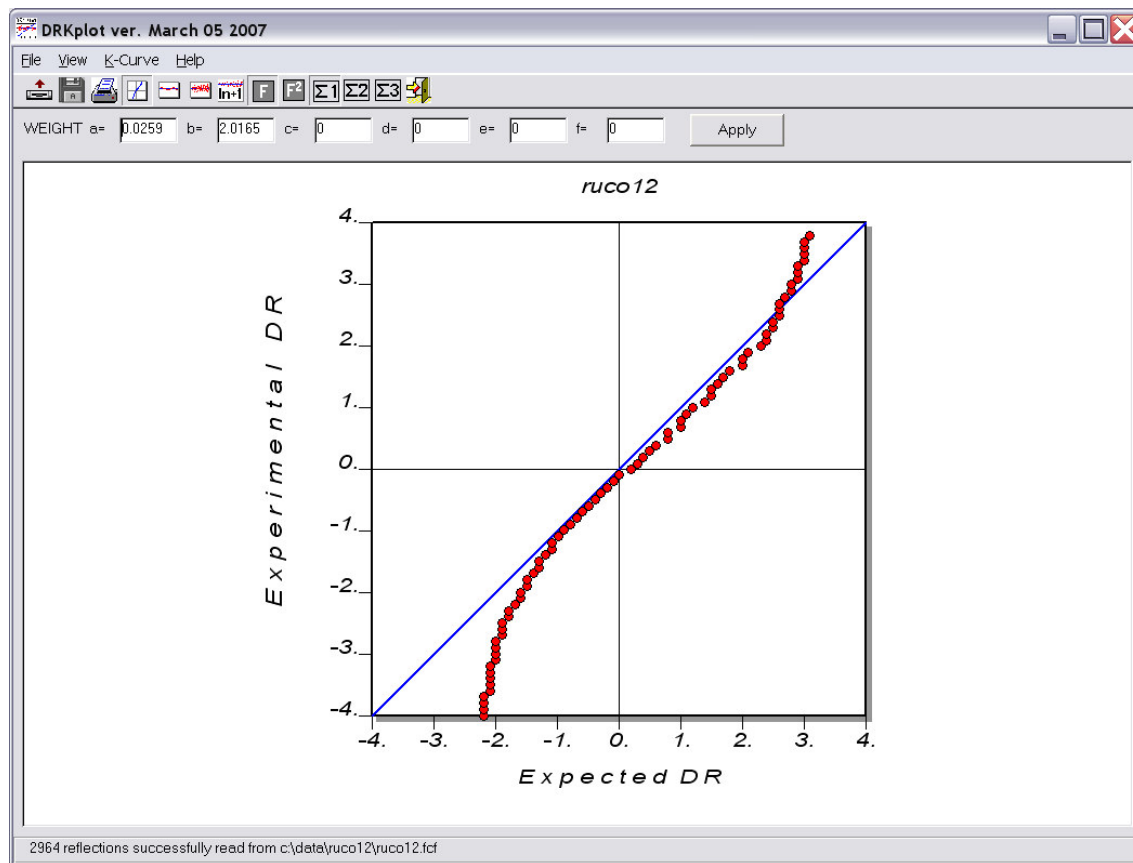
The second plot shows the individual scale factors F_{obs}/F_{calc} versus resolution, and indicates that the scale factor is reasonably well determined across the resolution range.



Such information may be better illustrated as a binned plot, as below. This plot also shows the effects of extinction, as the (generally) highly intense low angle data are systematically slightly underestimated.



The DRK-Plot program, written by Adam Stash (Moscow), has been included in WinGX by kind permission of the author. It duplicates to a certain extent the functionalities of Fo-Fc Plots, but has the additional capability of displaying the normal probability distribution plots of Abrahams and Keve [1] shown below.



These plots are of the experimental δR , *i.e.* $\Delta F/\sigma(F)$ versus values expected on the basis of a normal (Gaussian) distributions. The plots should be a straight line of unit slope if the errors are normally distributed and the experimental sigma's are appropriate. For further details of the interpretation of these plots, see [1].

1. Abrahams, S. C.; Keve, E. T. (1971) *Acta Cryst.* **A27**, 157.