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 <u>http://www.dplot.com/</u>,

or as a free cut-down version for just viewing the graphs from http://www.dplot.com/dplotviewer_setup.exe

III Fo-Fc Plots		
File		
Fo-Fc Data Plotting options		1
Fo-Fc file : list4.fcf		Browse
Fc-Fo format : SHELXL LIST4 FC	Ffile	
WEIGHT 0.0288 2.6685 0.00	00 0.0000 0.0000 0.3333	
Number of reflections is 3881, of	which 3640 were observed (F	o > 4.0*sigFo)
Sigma of electron density = 0.05	9 eA-3	
R-values		
The R-values calculated from t		
They are computed according identical, especially regarding		
reads any SHELXL FCF file whi	-	
will only agree with the SHELXL	output if the LIST 4 format is	used.
- SHELXL convention		
R1(obs) = 0.0225 R	1(all) = 0.0247 wR	= 0.0284
	2(all) = 0.0349 wR3	2 = 0.0652
_XD convention		
R{F} = 0.0225 R	all{F} = 0.0263 Rw4	F} = 0.0390
R{F^2} = 0.0347 R	all{F^2} = 0.0349 Rw	(F^2) = 0.0642
	Diet En En wordt	
	<u>P</u> lot Fo-Fc graph	<u>Cancel</u>

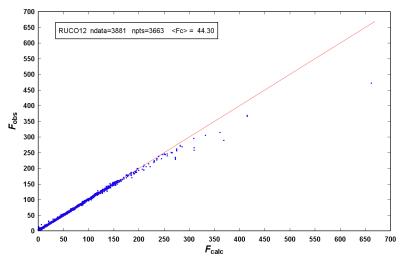
A number of standard R values are computed, according to the conventions of data treatement in SHELXL and XD. As well as reading the FCF file, the program attempts to obtain further information from a *name.INS* file (if SHELXL FCF file is input) or from *XD.MAS* if an XD.FCO file is loaded, regarding 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 *Fobs* vs *Fcalc* to show up the presence of extinction effects, or of *Fobs* vs $sin\theta/\lambda$ to determine whether the scale factor is linear across the resolution ranges

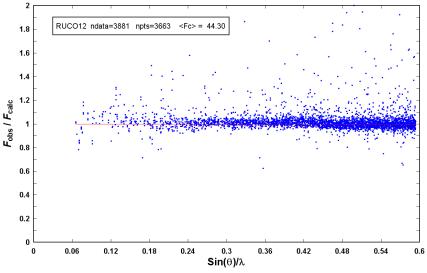
Fcalc min : 0.05 Options F/sigF min : 3 Plot reflection data as F^2 rather than F Include reflections flagged as "unobserve Send processing output to text server N_bin 50 Isplay data as a scatter plot Delta U 0 Display data as a binned plot Wavelength 0.71073 Use equally incremented bins	- Y-axis (ordi Fobs Fcalc Fobs/Fc Sig(Fob Innear sc Cogarithr	C Fobs C (Fob alc C (Fob s) C Fobs	s - Fcalc s - Fcalc)/Fcalc s - Fcalc)/sigFobs s/sigFobs	X-axis (abscissa) F(obs) F(calc) Sin(theta)/lamb Sig(Fobs) Ingarithmic sca
Use binning formula to minimise outliers	Plot title : Fcalc min : F/sigF min : N_bin Delta U Wavelength	3 50 0	 Plot reflection d Include reflectio Send processin Display data as Display data as Use equally po Use equally inc 	ns flagged as "unobserv g output to text server a scatter plot a binned plot pulated bins remented bins

Sample plots are :

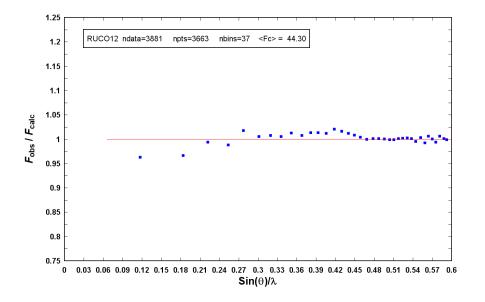


This plot clearly shows that the most intense reflections are consistently underestimated, which is indicative of extinction effects

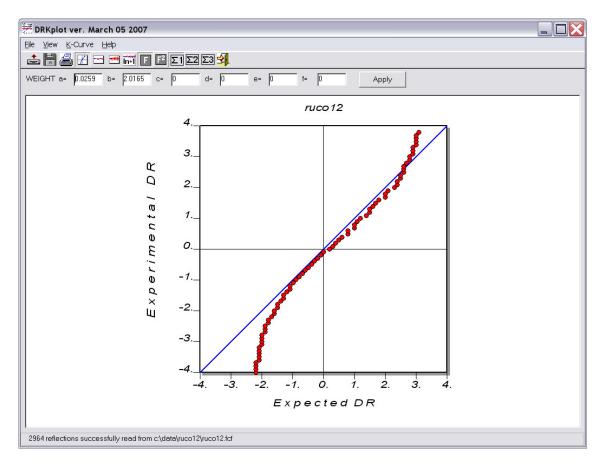
The second plot shows the individual scale factors F_{obs}/F_{calc} versus resolution, and indicates that the scale factor is reasonably well determined across the resolution range.



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.