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ANALYSIS OF TIME-OF-FLIGHT DIFFRACTION DATA FROM LIQUID AND AMORPHOUS SAMPLES

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INTRODUCTION

The purpose of this manual is to describe a package of data analysis routines which have been developed at the Rutherford Appleton Laboratory for the analysis of time-of-flight diffraction data from liquids, gases, and amorphous materials. It seemed to us that a majority of users were put off analysing their data properly because of the apparent complexity of TOF data, although in actual fact the basic steps are the same as in a reactor experiment. Furthermore our experience to date has shown that there really is no fundamental barrier to diffraction data being accurately analysed to structure factor or even pair correlation function within a very short time of the completion of the experiment (always assuming the computer is "up" of course!). What has prevented this in the past has been a lack of understanding of what to do with the data and how to do it. For our part the relevant routines have been spread around different directories with different modes of input and operation, which has led to great inefficiencies for all concerned.

Therefore the package has now been set up with all the relevant routines in a single area of the computer in such a way that it requires a minimum of understanding of computing aspects on the part of the users, at the same time as allowing them to check that each stage of the analysis has been completed satisfactorily, and also enabling them to re-sequence the steps or add additional ones according to their own requirements. For example application of inelasticity corrections and calculation of the pair correlation function tend to be controversial stages with each user having his or her own preferences for how they should be achieved. While the package supplies suitable routines, the users can readily incorporate their own preferred routines as necessary. At several points the package requires an intelligent interaction with the user which means he or she is not entirely free from responsibilities. Hopefully after studying this manual he or she will be able to respond to the requests made of him confidently!

The other guiding principle we have adopted is that the users will not be willing to ship the very large raw data files generated in these experiments, but on the other hand will be willing to remain a short while at RAL after their experiments in order to complete the routine analysis. In this way they can return home with the much smaller files containing the structural information they are seeking for more detailed manipulations at their home institutions. This makes sense because most university users are not equipped to handle the size of typical ISIS data files, nor provide the necessary archive which is done at ISIS immediately after each run is completed. Having said that however we also request that users do NOT use the ISIS HUB computer for these subsequent manipulations because by doing so they simply slow down the HUB for other users, who also can only afford to spend a limited time at RAL analysing their data. Of course there are no restrictions on those users ambitious enough to take the raw data home and analyse it from scratch themselves: we will be happy to let such people have copies of any of our routines that they might need.

The package has been developed primarily for analysis of ISIS data, but is not limited to a specific instrument: the procedures will work equally well on any ISIS diffractometer, although LAD is used as the example throughout this manual. Because of its great versatility the GENIE command language, invented by Bill David, or variants of it, is used for the main stages. However the only stage which is strictly ISIS specific is the very first in which the raw data in ISIS format are converted into GENIE format. Therefore the package could in principle be used at other institutions which have the GENIE language, the only modification required being to the initial input of the raw TOF data.

Obviously while every effort has been made to ensure that the routines do what we say they do, we can accept no responsibility for errors which may occur: careful checking at each stage normally should show up any errors. We would welcome suggestions for ways in which the procedures can be corrected and improved.

This manual is in no way comprehensive. Further details are contained in the papers referred to. In particular the reader is encouraged to read Colin Windsor's book, "Pulsed Neutron Scattering" [1].