# Instructions for rdf2ioq Small Particle Modeling Software

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*Alex Hannon*

## rdf2ioq

The main aim of the program rdf2ioq is to calculate the distinct scattering, *i(Q)*, that would be observed for a small particle of given structure.

The essential input to the program rdf2ioq is a .RDF file produced by the program XTAL.[1] Currently there are three ways in which this can be done:

1. The distinct scattering for a spherical particle of diameter *D* can be calculated as follows:
    a. Firstly, run XTAL using a large enough number of layers to give a maximum reliable distance which is larger than *D*. The maximum distance to which the correlation functions are calculated should also exceed *D*. It is essential that a .RDF file is produced.
    b. Secondly, run rdf2ioq on the .RDF file, and choose the option to apply the Mason spherical particle correction.[2] With this method, no explicit assumption is made about what atoms are at the surface of the sphere, but in effect for each partial function, the origin atom type is at the centre of the sphere. With this approach it is possible to subtract the small angle scattering contribution from the result. This is conceptually equivalent to surrounding the small particle with a uniform medium of the same density as the particle.
2. The distinct scattering for a cluster of unit cells can be calculated as follows:
    a. Firstly, run XTAL and specify the required number of layers for the model. (In this case, the model is made by surrounding a central unit cell with the requested number, $N_{layers}$, of layers. Thus the number of unit cells in the model is 1, or 27, or 64…etc.) Make a note of the length of the cell diagonal reported by XTAL. Choose the option to save the coordinated of the model in a .COORDS file.
    b. Secondly, run the program coords2atoms to convert the .COORDS file into a .XTAL file. It is strongly recommended to use a new name for the .XTAL file. This new .XTAL file will be for a molecular model, not a crystalline model.
    c. Thirdly, run XTAL again on the new .XTAL file to calculate the correlation functions up to a distance $r_{max}$ which must exceed the longest distance in the model (=$(2N_{layers}+1)$*length of cell diagonal).
    d. Finally, run rdf2ioq on the new .RDF file, and do not apply a small particle correction (because the model is already a small particle).
3. The user can calculate the distinct scattering for their own cluster model as follows:
    a. Firstly, generate the coordinates of the atoms in the model and put them in a .XTAL file to make a molecular model (see the XTAL manual[1] for details).
    b. Secondly, run XTAL to calculate the correlation functions, using a maximum distance, $r_{max}$, which is larger than the largest interatomic distance in the model.
    c. Thirdly, run rdf2ioq on the .RDF file.

The program rdf2ioq performs essentially almost the same calculation as the Debye equation. However, it can be much more efficient for larger models than direct use of the Debye equation, and so the program is much faster.

An advantage of the program rdf2ioq is that it correctly takes into account partial occupancies. This is done by appropriate weighting of each atomic site with a partial occupancy, rather than assuming any particular arrangement of the partially occupied sites.

The variation with distance of the RMS thermal variation in interatomic distance, $\langle u^2 \rangle^{½}$, can be described in a number of ways. It is recommended that a physically realistic set of thermal parameters be used, which gives a realistic description of the measured correlation function.

The result of the program rdf2ioq is stored in a .IOQ program which can be read in to OpenGenie. If the calculation is scaled for either neutron or X-ray diffraction, then the last block of the file contains the calculated total function (the appropriately weighted sum of all the partial functions).

**References**

1. Hannon, A. C., *XTAL: A program for calculating interatomic distances and coordination numbers for model structures,* Report RAL-93-063, 1993.
2. Mason, G. *Nature,* 1968, **217**, 733.