XTAL Correlation Function Simulation Software

The XTAL programs provide a means of taking an atomic structure model and calculating the correlation functions, and also determining the structural properties of the model.

The original reference for the XTAL software is:
A.C. Hannon, *XTAL: A program for calculating interatomic distances and coordination numbers for model structures*, Rutherford Appleton Laboratory Report RAL-93-063, 1993.

The original reference for the XTAL software may be downloaded here: XTAL manual RAL-03-063 report.pdf

The Windows version of the XTAL software may be downloaded here: xtal.zip The files must be downloaded to the correct directory.

Here are descriptions of the Windows software:

Program	*Purpose*	*Input*	*Output*
MAKEX	Generate input file for XTAL from crystal structure file	`.XREF` or `.CIF` file	`.XTAL` file `.URMS` file
XTAL	Calculate partial correlation functions for model structure. Search for interatomic distances. Calculate coordination numbers. Determine bond angles. Calculate polyhedral distortion.	`.XTAL` file	`.RDF` file `.ANA` file `.BAN` file `.PAN` file
RDF	Broaden correlation functions of model	`.RDF` file `.URMS` file	Genie workspaces
COORDS2ATOMS	Convert atomic coordinate datafile into ATOMS plot file or `.CHEM3D` file for CrystalMaker	`.COORDS` or `.CFG` file or `.ATO` or `.PDB` file	`.STR` file or `.CHEM3D` file

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MakeX

MakeX is used to make a `.XTAL` file for input to the XTAL program. The `.XTAL` file is a description of the structure of a model (crystalline or molecular) from which XTAL can calculate the correlation functions, and other structural parameters.

It is recommended to run MakeX from a command prompt window (not by double-clicking an icon) because the output can be followed better in this way.

MakeX is designed specifically to produce `.XTAL` files for crystalline models, using an input file from a crystal structure database.

The input to MakeX is either a `.CIF` file or a `.XREF` file. Both of these may be generated from the ICSD database by using the Chemical Database Service interface. A `.CIF` file is generated by using the web interface to ICSD, whilst a `.XREF` file is generated by using the command line interface to ICSD.

The contents of a `.XTAL` file are described in the original XTAL manual : XTAL manual RAL-03-063 report.pdf

MakeX can also use the crystallographic thermal parameters in a .CIF file to produce a .URMS file which contains the rms variation in bond length for each partial correlation function. This can be used by the RDF program to broaden the model correlation functions for the effect of atomic thermal motions.

A version list for MakeX is here.

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The XTAL Program

The principal task of the XTAL program is to calculate radial distribution functions for atomic structure models.

The program can also be used to perform the following calculations...

- Determine the coordination number of the atoms in the structure
- Find which atom pairs have a separation within a specified range
- Determine the bond angles of the structure
- Calculate the distortion of the polyhedra in the structure

It is recommended to run XTAL from a command prompt window (not by double-clicking an icon) because the output can be followed better in this way.

The input to the XTAL is a `.XTAL` file. This can be created manually by following the description in XTAL manual RAL-03-063 report.pdf. Or for a crystalline model it can be generated automatically using the MAKEX program on a file from a crystal structure database.

The principal output from XTAL is a `.RDF` file, which contains the partial radial distribution functions for the model.

The correlation functions calculated by XTAL are not broadened for the effects of thermal motion or real-space resolution - this broadening can be done by using the RDF program.

A version list for XTAL is here.

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RDF

RDF is used to broaden the partial correlation functions of a model for the effects of thermal atomic motion and real-space resolution. It requires a `.RDF` file as input, and hence it must be run after running the XTAL program.

RDF can only be run from within OpenGenie, and furthermore it will only run successfully if the GEMSQRAW suite of programs has been installed.

To use RDF you must type **`load "c:\g_f\rdf.gcl"`** after starting OpenGenie. Then the program will run every time you type **`rdf`**.

The algorithm used can in principle only broaden the model correlation functions for the effects of both thermal atomic motion and real-space resolution. If you wish to broaden for real-space resolution only, then set the atomic displacement to zero. It is not possible to broaden for thermal motion only, but if Q_{max} is set to a large value, say 100Å^{-1} or greater, then the effect of real-space resolution can be made small.

If more than one different value is required for the atomic displacement, *u*, then the values must be specified using a `.URMS` file. Here is an example of a `.URMS` file for a model with 2 atom types...

```
5
1 1 1 1 0.16
1 2 1 2 0.05 2.0 0.16
2 1 1 2 0.05 2.0 0.16
2 2 1 1 0.16
0 0 1 1 0.05
```

The first record gives the number of correlation functions - in this case there are 4 partial functions, and also a total function.

The subsequent records start with origin atom type, and second atom type - note that the partials must follow the order given in the example.

The 3rd value is the broadening mode. Currently three broadening modes are provided, as described below.

In this way, different ranges in *r* can be broadened with different values of the atomic displacement, *u*. And different partial functions can be broadened with different values of *u* too.

The MakeX program can be used to generate a `.URMS` file for which the RMS bond length variations are calculated from the crystallographic thermal parameters in the `.CIF` file.

Broadening mode 1

> For mode 1 there are constant values of *u*, each over a distance range, specified by break-points. The 4th value is the number of distance ranges. The 5th value is the value of *u* for short distances. This is followed by the value of *r* for the first break-point. Next comes the value of *u* for distances longer than the first break-point, and so on.
>
> e.g.
> `1 2 1 2 0.05 2.0 0.16`
>
> For this example, the 1-2 correlation function is broadened with *u*=0.05Å for distances less than 2.0Å, and then longer distances are broadened with *u*=0.16Å.

Broadening mode 2

For mode 2 the low-*r* region is divided into ranges with constant values of *u*, the same as for mode 1. Then the final high-*r* region has an *r*-dependent value of *u*, according to the following equation

$$\langle u^2 \rangle^{½} = \sqrt{\langle u^2 \rangle_0 - \frac{\delta_1}{r} - \frac{\delta_2}{r^2}}$$

Three values (u_0, δ_1, δ_2) are then given to specify *u* for high-*r*. u_0 is the limiting value of *u*, for very long distances. Note that δ_1 is usually set to zero.

If the number of regions is one, then there is no region with a constant value of *u*.

e.g.

```
2 2 2 2 0.07 2.5 0.19 0.0 0.1
```

For this example, the 2-2 correlation function is broadened with *u*=0.07Å for distances less than 2.5Å, and then longer distances are broadened with $u=(0.19–0.1/r^2)^{½}$.

Broadening mode 3

For mode 3 the low-*r* region is divided into ranges with constant values of *u*, the same as for mode 1. Then the final high-*r* region has an *r*-dependent value of *u*, which is determined according to the correlated Debye model (*Jeong et al, Phys Rev B 67(2003)104301*)

7 values (T, M_1, M_2, θ_{D1}, θ_{D2}, k_{D1}, k_{D2}) are then given to specify *u* for high-*r*. *T* is the temperature in Kelvin, M_1 and M_2 are the atomic masses in amu of the elements involved in the partial, θ_{D1} and θ_{D2} are the Debye temperatures in Kelvin for the elements involved in the partial, and k_{D1} and k_{D2} are the Debye wavevectors in $Å^{-1}$ for the elements involved in the partial.

If the number of regions is one, then there is no region with a constant value of *u*.

e.g.

```
2 2 3 2 0.05 1.9 293.0 72.59 15.9994 307.0 307.0 1.556 1.556
```

For this example, the 2-2 correlation function is broadened with *u*=0.05Å for distances less than 1.9Å, and then longer distances are broadened with a thermal width $u = \left(u_1^2 + u_2^2\right)^{½}$, where the mean square displacement of element 1 is calculated according to the correlated Debye model, with temperature *T*=293K, mass M_1,=72.59amu, Debye Temperature θ_{D1}=307K, and Debye wavevector k_{D1}=1.556 $Å^{-1}$.

A version list for RDF is here.

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The coords2atoms Program

The coords2atoms program may be used to convert a file containing the coordinates etc for a model from one type to another type.

The following types of input file can be used:

Input file type	*description*
.COORDS	Traditional coordinates file
.CFG	RMC file
.ATO	EPSR file
.PDB	Protein DataBank file

The following types of input file can be made:

Output file type	*description*
.XTAL	For use by XTAL
.ATM	For importing coordinates to ATOMS plotting software
.CHEM3D	Useful for importing a model to CrystalMaker plotting software
.STR	For use by ATOMS plotting software

A version list for coords2atoms is here.

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