ZMCGUI v1.0 USER Manual

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Preface

ZMCGUIv1.0 is a prototype for a user friendly interface that allows one to quickly load up molecular crystal structure models into a Monte Carlo atomistic simulation program and perform calculations of scattered intensities projected in K-space. The major driving force for development of this GUI was that most approaches to study of X-ray diffuse scattering from molecular crystals, through the use of atomistic MC simulations are performed using custom-built or ad-hoc software. The ZMCGUI is an attempt to generalize this procedure when working with molecular crystalline systems.

ZMCGUI currently takes the form of a python application - it is in development and still has many features that need to be added. In the current state ZMCGUI is not entirely stand alone and certain input files may still require some manual editing (we are constantly working to reduce this need).

The philosophy of ZMCGUI is to reduce the amount of manual editing that is required by user who just want to obtain rapid turnaround for what their diffraction data represents, and it is a good place to start to quickly generate the sets of input file you might use to setup your simulation experiments as well as DIFFUSE calculations.

ZMCGUI was designed with the intention that if you can grow a crystal, solve and refine the crystal structure, then you can also solve problems related to crystalline disorder. This simple set of GUI commands quickly enables encourages newcomers to the world of diffuse scattering. Professional users are also encouraged to use ZMCGUI with your other favorite crystallography or imaging software's, codes, etc. to solve problems and enhance workflows.

For more details on ZMC and DIFFUSE please refer to the respective user manual and literature articles.

1. Setup

Before Installation and running.

Currently In order to run this version of the ZMCGUI prototype you will need to have a working version of python 2.7 with openbabel python bindings correctly installed.

https://www.python.org/download/releases/2.7/

http://openbabel.org/wiki/Main_Page

Use of ZMCGUI is greatly facilitated by having a working version of the program mercury (the features in the free version are all that is required) to perform conversion of models into the .mol2 format which is required as the starting point for operation.

http://www.ccdc.cam.ac.uk/solutions/csd-system/components/mercury/

This program facilitates creating the .mol2 file which is needed for input(we provide examples of these in the ./example_structures/ directory) is a really great tool for working and visualization of molecular crystals.

In addition to python you will also need to make sure the python libraries numpy and matplotlib are setup correctly. Other than this the ZMCGUI set of tools is reasonably self-contained.

Environment

Please set appropriate environment variable for executables:

ZMCGUI_BIN=path\to\zmc_GUI\bin\

In the following document (.) refers to the zmc_GUI_distr path (i.e. the path this manual was in)

Running

Relevant gui files are in

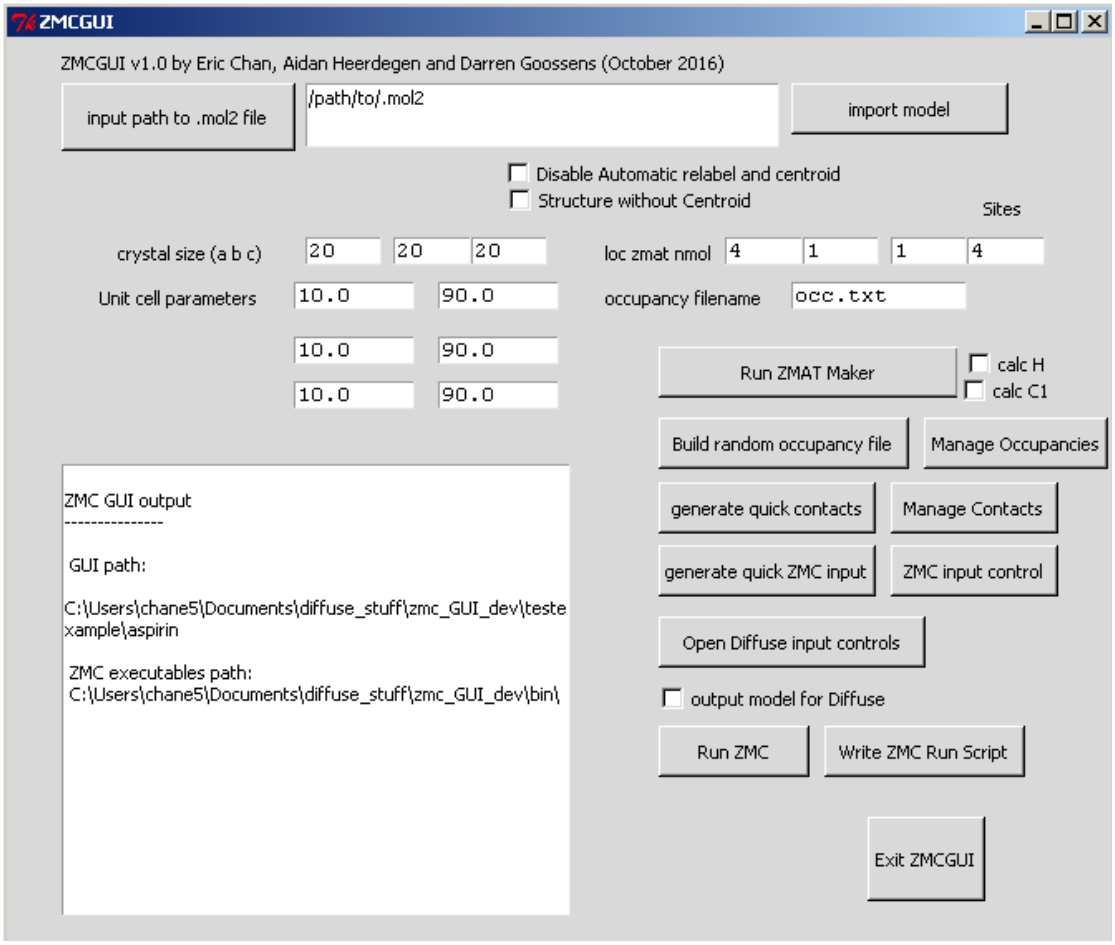
./page

once you have your python2.7 setup properly you can run the GUI from the command line using

python ZMCGUI.py

or you should be able to start by double clicking on ZMCGUI.py

2. Main Window Tasks



Task Button Descriptions

- Input path to .mol2 file: Brings up a file selection window so that the user can select the desired model in .mol2 format. When you click on this button it will bring up a file selection dialog and the user is directed to select the structure (.mol2) file.
- Import model: Reads the necessary data from the .mol2 file. This will run a routine that prepares the structure so it can be read by the ZMAT maker. There are two options which are used if you want to read in a .mol2 file that you have manually edited. *Disable automatic relabel and centroid (default unchecked)* : Check this to turn off the automated relabeling and centroid generation procedure. *Structure without centroid (default unchecked):* use this when there is no separate centroid in the .mol2 (see the urea example for more details) as long as this box is checked all inputs for procedures will assume there is no centroid.

  Important note: The procedure for importing models for automated relabeling is very sensitive to the syntax of the .mol2. The procedure will create a file which is named by default to be [rootname]_relabel.mol2 which you can check to see if the syntax is appropriate for zmat_maker

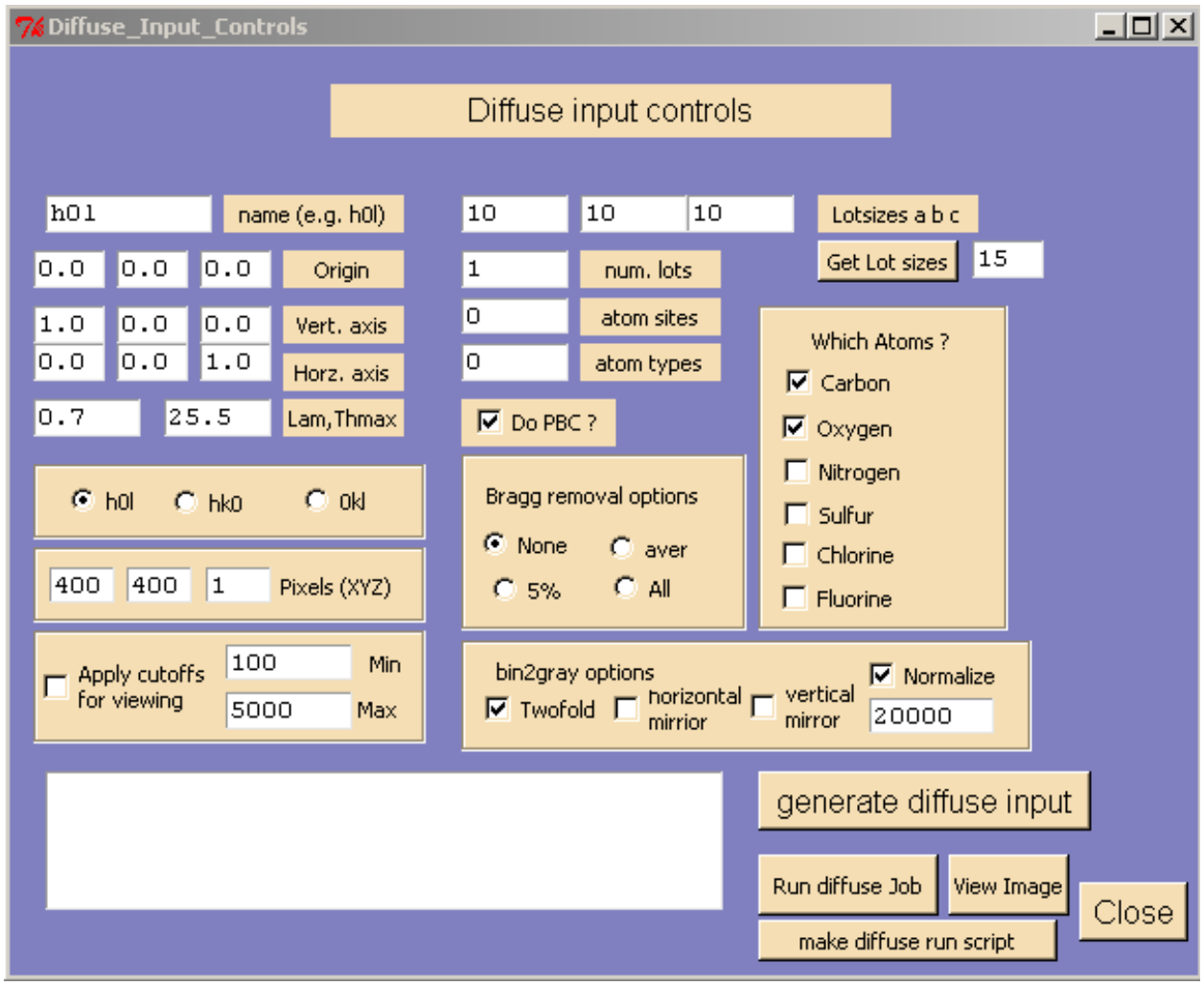
or even just load in mercury. If there is a problem try to remove the atom numbering scheme given in the original .cif file prior to exporting at the .mol2 for processing by ZMCGUI. Only atom names are needed by the program.

- Run ZMAT maker: Creates the files for Z-matrices (*.zmat) and quaternions (*.qxyz). This procedure will also initialize some variables such as location and Z-matrices. There are two options for ZMAT handling via checkboxes on the right of this button. *Calc H (default unchecked):* Check this to enable contribution from hydrogen atoms during a structure factor calculation. *Calc C1(default unchecked):* Check this when you want to enable contribution from the centroid atom during structure factor calculation (note: It is necessary to check this option when you have already checked 'Structure without centroid' option during the 'import model' task).
- Build random occupancy file: This runs a task to build the file with site occupancy Information that will be used by ZMC. If you have multiple Z-matrices they will be distributed randomly through the model crystal. The name of the output occupancy file will correspond to the name given in the 'occupancy filename' entry box. Advanced users can create the occupancy file manually and place corresponding names in the mentioned entry box so that other tasks can reference this name during running.
- Generate Quick Contacts: Generates and organizes a minimal list of intermolecular interactions used by the MC algorithm to determine atomic displacements during the simulation. The procedure is based on a method described in previous articles (Chan et. al.) and will automatically select the appropriate interactions and assign the required force constants.
- Generate quick ZMC Input: This task will generate a minimal ZMC input file for running ZMC. If this is the first run of ZMC for this structure in the chosen folder then you will need to make sure all the other relevant files are available (i.e. Z-matrices, occupancies, contacts). This is possible using the previous tasks described.
- Manage Occupancies: Opens the manage occupancies dialog window.
- Manage contacts: Opens the manage contacts dialog window.
- ZMC input control: Opens window for advanced ZMC input controls.
- Open Diffuse input controls: Opens window to diffuse input controls.
- Run ZMC: Runs the ZMC program using the available input files.
- Write ZMC Run Script: This outputs a python script that can be used to run ZMC remotely
- Exit ZMCGUI: Close and exit the GUI

Description of parameter entry boxes

- Crystal size (a b c): This is the simulation size in unit cells
- Unit cell parameters: 1st column of entries are the familiar lattice parameters a, b, c. The 2nd column are α, β and γ.
- Loc zmat nmol: The number of location in the unit cell; then number of z- matrices; the number of molecular configurations.

2. Diffuse Input control Tasks



Task Button descriptions

- Get lot sizes: Runs a simple diagnostic routine that calculates a list of possible lots sizes based on the input data. It is then up to the users discretion to select the desired lot size parameters. A standard criteria for the lot shape is cuboid, as deviation from such a neutral shape affects the shape of the calculated scattering centered at the Bragg peak position. Given a crystal structure in a standard setting with roughly orthogonal axis, the unit cell parameters can be used to approximate sets of possible lot shapes (i.e. lot sizes a, b and c in terms of unit cells). The entry box to the right allows the user to specify the number of iterations, where each iteration will increment possible lot sizes and also specify an appropriate number of lots (number of samples), to use for the diffuse calculation.

- Generate diffuse input: Creates the files needed to run a DIFFUSE calculation using the current input values given by the window. Hit this button before attempting to run a diffuse job
- Run diffuse Job: Runs the diffuse scattering calculation.
- View Image: View the image that you have just created.
- Make diffuse run script: Creates a python script which can be used to run the diffuse calculations from the OS command line.

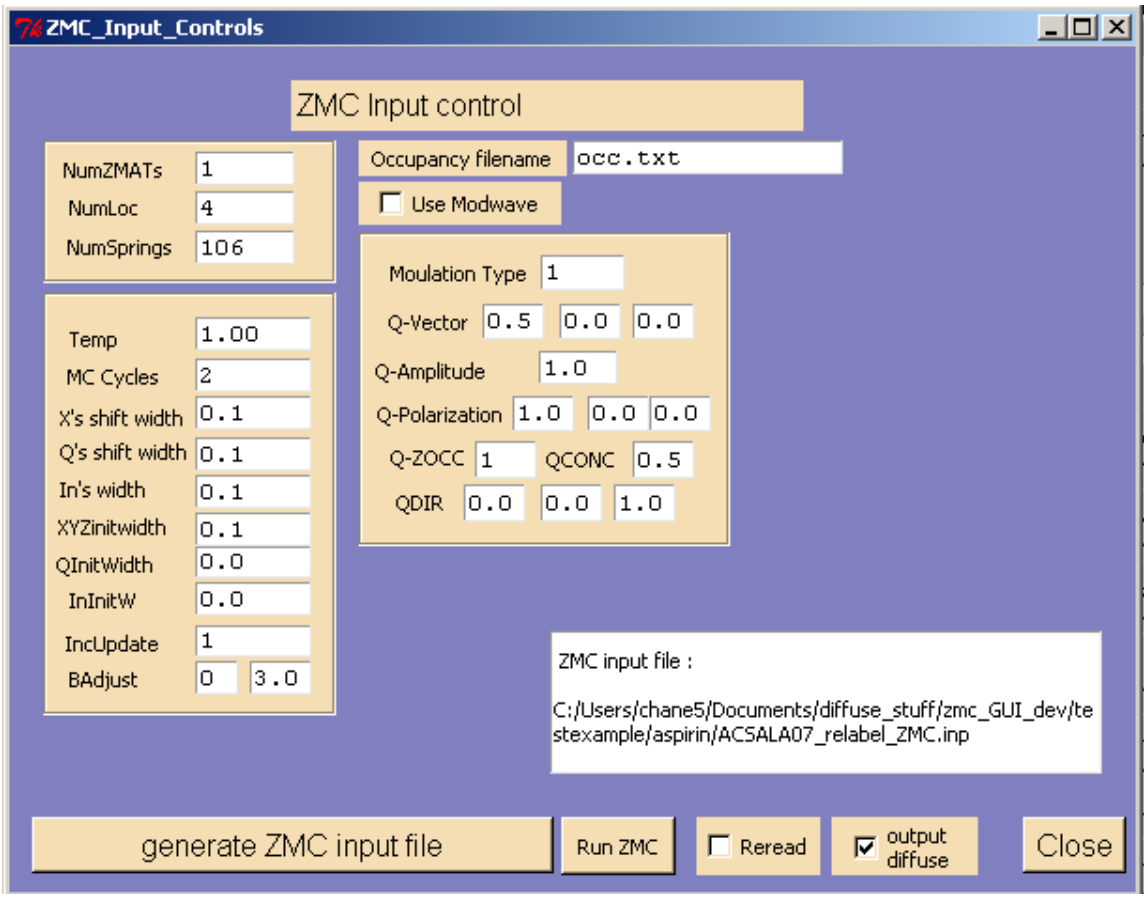
Radio Button and check box descriptions

- Basal sections h0l; hk0; 0kl: selecting any of these radio buttons will adjust the parameters for the origin, vertical and horizontal axes such that the reciprocal space section inputs specified can be generated and thus calculated and viewed. These radio buttons act as shortcuts so that the user can more easily generate and view diffuse input files for the basal sections.
- Bragg peak removal options: Select an option for how Bragg components are treated *None (default)* Do not remove Bragg component. *Average.* Remove Bragg peaks based on the average structure provided by a single unit cell. *5%* Average from 5% of the simulation to remove Bragg peaks. *All* Calculate average from the entire crystal (takes a long time).
- Which atoms: check the atom types you would like calculated (in most cases you will choose all relevant types for the molecule you are studying).
- Bin2Gray options: These option affect how the bin2gray.exe program is run. *Twofold.* Perform twofold averaging of intensities. . *Mirror.* Perform either horizontal or mirror averaging of the intensities. *Normalize.* Check this box to scale the intensities to the given value in the parameter box (default 20000).
- Apply cutoffs for viewing: Use parameter entries to allow for max and min intensity cutoffs when viewing projections.
- Do PBC: (default on) Check this box if the crystal simulation has periodic boundary conditions. If not the size of the calculation will be confined within boundary of the crystal (i.e. xtal_xyz – lot_zyz).

Description of parameter entry boxes

- Name: Name of the reciprocal space projection. Acts as the string indicator for each projection in the project (usually specified as crystal plane miller index)
- Origin: This is the center of the chosen reciprocal space projection.
- Vertical Axis: The vertical axis in reciprocal space expressed as a vector.
- Horizontal Axis: The horizontal axis in reciprocal space expressed as a vector.
- Lam, Thmax: The wavelength for the scattering radiation (Lambda). Diffraction angle, Theta Max.
- Pixels (xyz): number of pixels to be calculated in each dimension.
- Lot sizes (xyz): specify size of Lot in unit cells.
- Num. lots: Total number of lots to be calculated and averaged.
- Atom sites: Number of possible atom sites in the unit cell.
- Atom types: Number of possible atom types in the unit cell.

3. ZMC Input control Tasks



Task Button descriptions

- Generate ZMC input file: This generates the ZMC input file using the variables accessible in this input control window. The task requires that prior contacts data has been generated using either the "generate quick contacts" option from the main window or using the advanced contacts management options. It is mandatory to generate the input file from this window if the structure you are working with has multiple Z-matrices.
- Run ZMC: runs the ZMC program using the generated input and options provided by the checkboxes in this window.

Radio Button and check box descriptions

- Use Modwave: Check this box to implement the modulated structure generation options. When this box is checked along with the "output diffuse" option, ZMC is run twice. The initial run will implement structure modification according to "use modwave" options (described below), the final run will reread the structure and then output the model of diffuse coordinates. If you want

to perform multiple modulations then make use of the “reread” option and do not output diffuse.

- Reread: This rereads a previously generated ZMC *.crystal file into ZMC.
- Output diffuse: This outputs the ZMC *.diffuse file.

Description of parameter entry boxes

- NumZMATs: This is the number of Z-matrices. (Known Bug: In some cases ZMC requires that for each ZMAT a line NUMINTERNAL is also specified. The bug was identified with command line based ZMC input construction and has not currently been observed with use of the GUI)
- NumLoc: Number of locations in the unit cell.
- NumSprings: Number of springs.
- Temp: Simulation temperature (relative to KT).
- MC cycles: Number of Monte Carlo cycles.
- X’s shift width: Positional shift increment width.
- Q’s shift width: Quaternion shift increment width.
- In’s width: Internal DOF shift width.
- XYZinitwidth: Positional displacement when initializing the crystal.
- QInitWidth: Orientation displacement when initializing the crystal.
- InInitW: Internal DOF when initializing the crystal.
- IncUpdate: Toggles how often (no. of cycles) increments will be rescaled so that MC acceptance ratios are close to 0.5. Shifts on variables are adjusted so that they have equal influence on the acceptance ratio.
- BAdjust: Scale spring constants so that the simulation displacements will have a distribution likened to a particular Debye-Waller factor.
- Modulation Type: Integer value which specifies the type of modulation 1. Displacement, 2. Occupancy, 3 orientation.
- Q-vector: .3 component vector which specifies the direction of the modulation
- Q-amplitude: Magnitude of the modulation.
- Q-polarization: Polarization vector.
- Q-ZOCC: Z-matrices that are affected.
- QCONC: Concentration.
- QDIR: Direction for orientation modulation.

4. Step by Step examples

The expected output files (with the exception of *.diffuse and *.crystal), for the examples described in this document, from the stable distribution are packaged with the setup files (i.e. ZMCGUI.zip) and can be found in the ./zmc_GUI/testexamples directory. After you go through the examples listed here, Please try out ZMCGUI using the other molecular crystal examples provided. Have fun.

Aspirin example

1. Make a new directory somewhere on your local drive and copy over the example structure files

$>mkdir aspirin

$>cp example_structures/ACSALA07.mol2 aspirin/.

or

1.1 Open the example_structures/ACSALA07.cif in mercury

1.2 In the lower left-hand side of the mercury window - click the "packing" checkbox then go file->SaveAs

1.3 Save the file in the aspirin directory in .mol2 format

1.4 Close mercury

2. Open the ZMCGUI as described above

3. Click "input path to .mol2 file", select the ACSALA07.mol2, open, then click "import model" ZMCGUI will load up the .mol2 file and prepare it for zmatmaker. you can follow the output to check that everything went ok.

4. Click "Run ZMAT Maker" to create .zmat and .qxyz files.

5. In the following sequence click "Build random occupancy file", "generate quick contacts", "generate quick ZMC input".

6. Check the box "output model for diffuse".

7. Click "Run ZMC".

If you have made it this far, well done, you have just made yourself a nanoscale simulation of an aspirin crystal.

Now quickly calculate what the Bragg diffraction looks like

8. Click "diffuse input controls" to open the diffuse input dialog

9. For now we will just leave the Lot sizes alone at the bottom right hand corner click the button "generate diffuse input" this will generate the diffuse input file required for calculating a h0l section given the specified settings

10 click "run diffuse job"

11. To see the .pgm image click "View Image"

12. Close the image by clicking the 'X' in the top right hand corner of the image window.

13. Now click the radio button that is labeled "hk0" notice you will see some options change.

14. By using the radio buttons "hk0" and "0kl" repeat the process "generate diffuse input" and "Run diffuse Job" to generate corresponding .pgm images

15. You may view the images by clicking "View Image" making sure that the name box (top left) has the correct label that you want to see. This is more easily done using the radio button but will only work for basal planes.

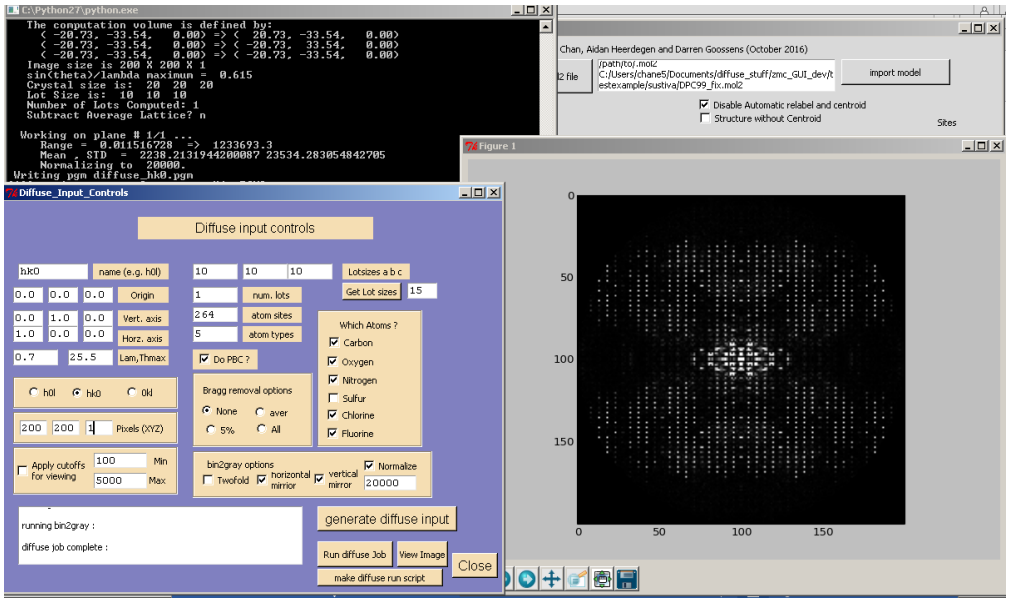
"well done" - you have just used both ZMC and DIFFUSE to calculation a diffraction pattern

If you repeat roughly the same procedure for your own model you will be a step closer towards rapidly develop skills to solving your own diffuse scattering problem.

Suggestion: try a much larger simulation with more MC cycles parameters and calculate only the diffuse contribution averaging over many more lots sizes and compare the results. You may like to use the “Write ZMC run script” and “write Diffuse run script” to help you do this.

Sustiva example (reading in a manually edited .mol2 file)

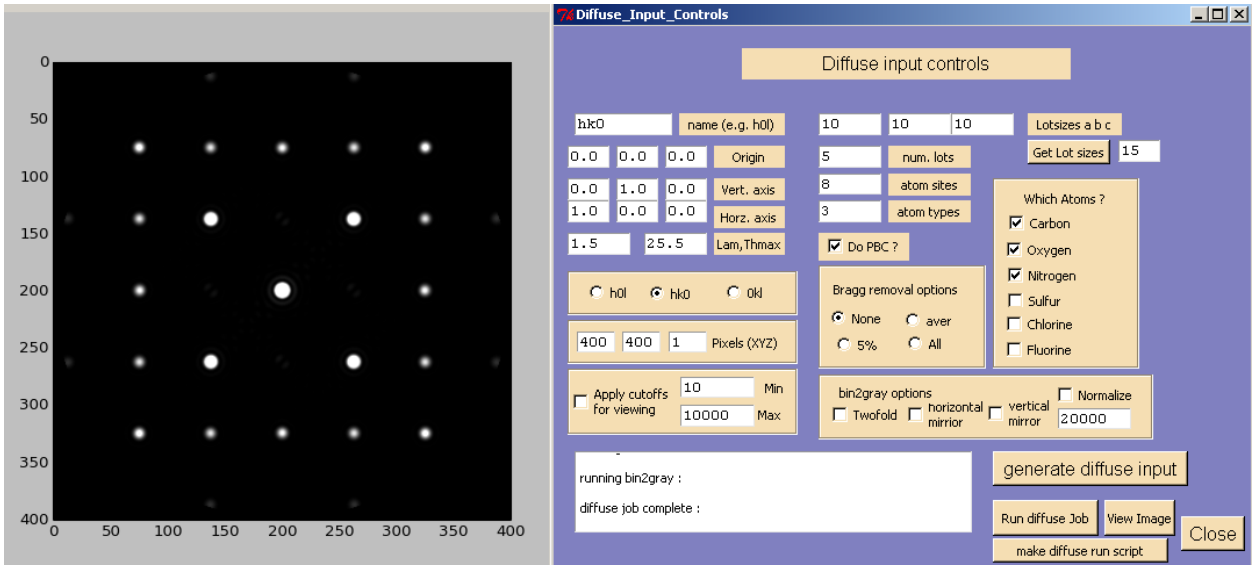
1. Make yourself a working directory called “sustiva”, then copy over the file DPC99190.cif and follow the steps 1-4 as per the aspirin example above. In the console widow you will notice the running of ZMAT maker will return an error. This is a known feature of the program zmat_maker and means the .mol2 file has to be manually edited before it can be successfully converted into Z-matricies.
2. Copy over the .mol2 DPC99_fix.mol2 from the example list. This file has been appropriately modified so that it will work using ZMCGUI.
3. Click "input path to .mol2 file", select the ACSALA07.mol2, open, make sure the check box “*Disable automatic relabel and centroid* ” is checked , then click "import model" ZMCGUI will load up the .mol2 file and prepare it for zmatmaker. you can follow the output to check that everything went ok.
4. Click "Run ZMAT Maker" to create .zmat and .qxyz files.
5. In the following sequence click "Build random occupancy file" then "generate quick contacts".
6. Click “ZMC input control”
7. From the ZMC input control window click “generate ZMC input file” then “Run ZMC” to run the ZMC program.
8. From the ZMCGUI main window click “open diffuse input controls”.
9. Using the diffuse input control window select the radio button “hk0”.
10. Under which atoms? Select all atoms except sulfur.
11. In the first two pixels(XYZ) entry boxes change both values to “200” (this will speed up the calculation, just so you can see that it works).
12. Under “bin2gray options” deselect “twofold” and select both “horizontal” and “vertical” mirrors.
13. Click “generate diffuse input” followed by “run diffuse job”
14. Once the job is complete. Click view image to see the image (below).



Urea example (structure without centroid and modulation example)*

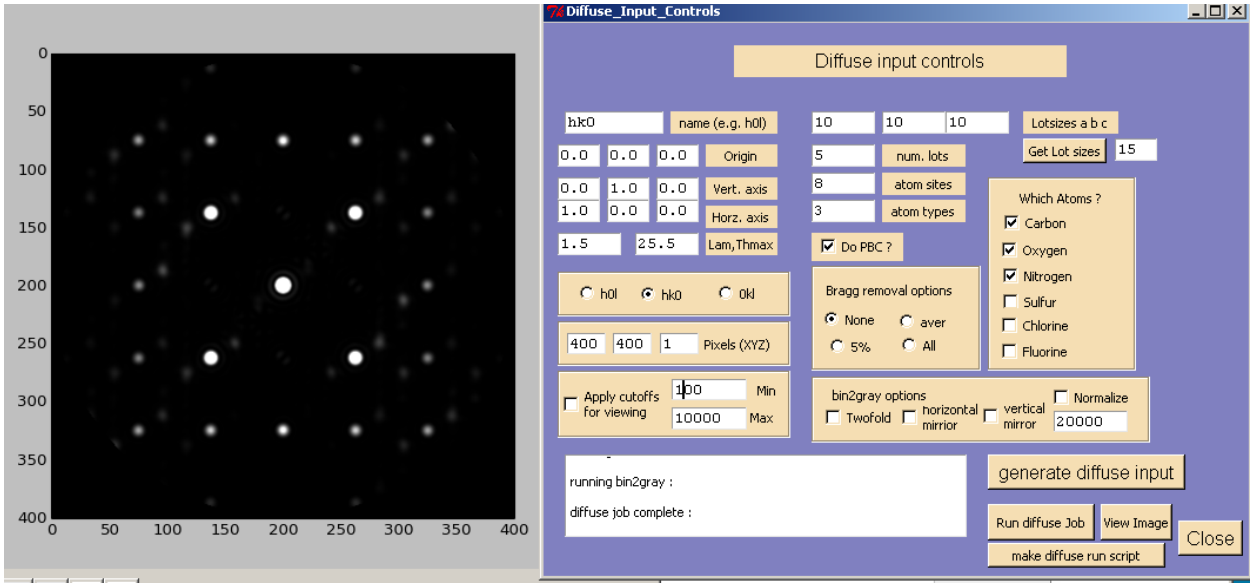
*note: Tetragonal urea is not a modulated structure we are just using this as an example to show how you can use the ZMC program to create modulated structures.

1. Make yourself a working directory called “urea”, then copy over the file urea.mol2 from the example files directory. This file has been manually modified in a fashion similar to early days of ZMC usage.
2. Click "input path to .mol2 file", select the ACSALA07.mol2, open, make sure the check boxes “*Disable automatic relabel and centroid* ” and “structure without centroid” are checked , then click "import model" ZMCGUI will load up the .mol2 file and prepare it for zmatmaker. you can follow the output to check that everything went ok.
3. Run the task “zmatmaker” making sure the “calc C1” box is checked,
4. Run the tasks “make occupancy” and ”generate quick contacts” from the ZMCGUI Main window.
5. Open both “ZMC input controls” and “DIFFUSE input controls”.
6. From the ZMC input control menu. Change “MC cycles” to 1.0. click “generate ZMC input file” then click “run ZMC”
7. From “diffuse input control” click “hk0”. Set atoms to Carbon, Oxygen and Nitrogen. Set “number of lots” to 5. Set Lambda to 1.5. uncheck “twofold” and “Normalize” in the bin2gray options.
8. Click “generate diffuse input” and then “run diffuse job” since you are doing 5 lots it may take a while longer.
9. Once the job is complete, take a look at the hk0 section by clicking “view image” (see below image for output).

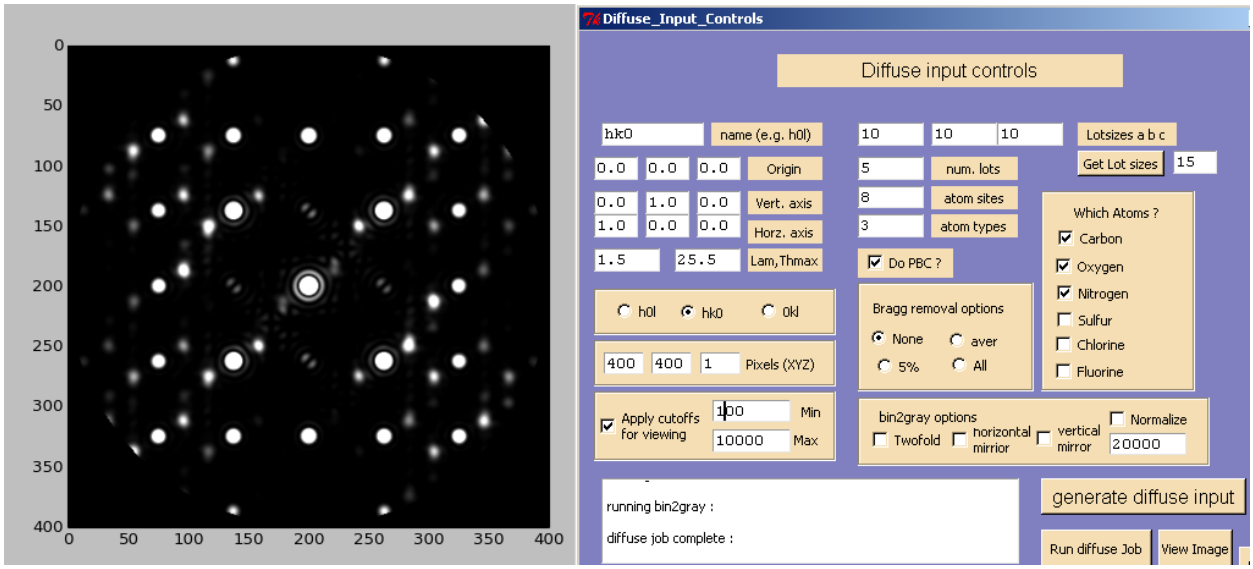


10. Now go back to the ZMC input control menu
11. Check the box “use modwave”, Set modulation type to 1. Set Q-vector to [0.33,0.22,0.0], set Q-Amplitude to 0.5, set Q-polarization to [1.0,0.0,0.0]

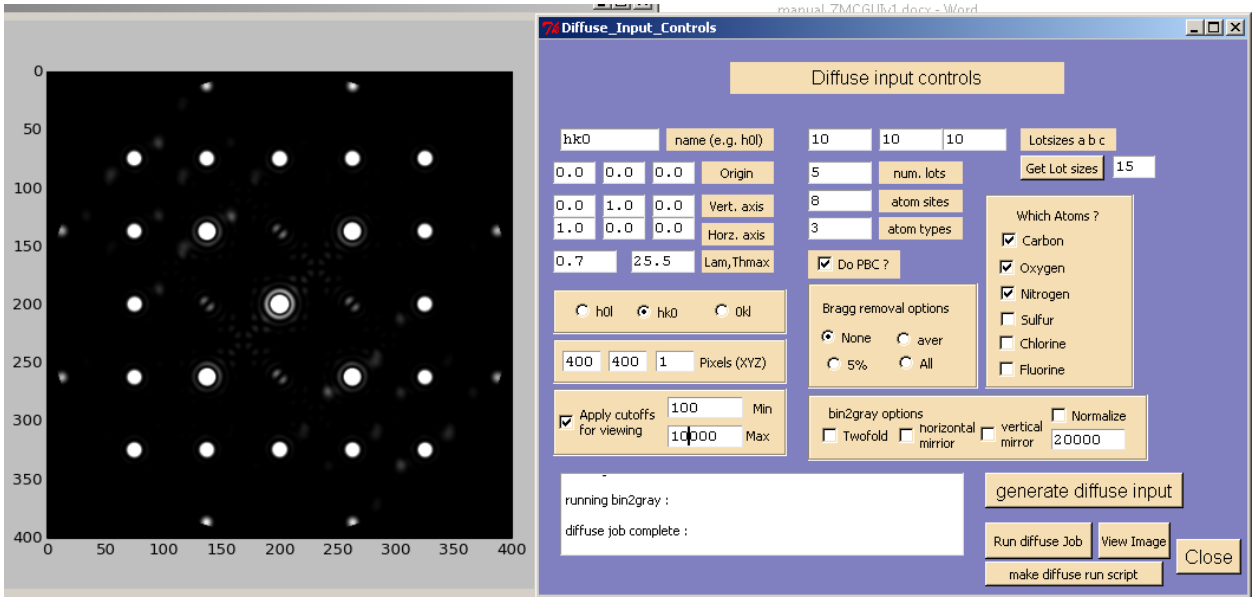
12. Check the box “output diffuse” then click “generate ZMC input file” then “Run ZMC”.
13. Once ZMC has finished, go to “diffuse input control window” and click run diffuse job.
14. Once this has finished, Click view image. If you did everything correctly, you should see the below image, notice in comparison to the other image the faint inter-modulation satellites.



15. Under diffuse input controls, check the box “apply cutoffs for viewing” , set “min” to “100” and “max” to “10000“ , then click the “view image button” you should see the below image, notice in comparison to the other image the inter-modulation satellites are clearly more pronounced and there are some other features which are artifacts from the calculation.



16. Now go to “ZMC input controls “.make sure the “use modwave” box is unchecked. Check the box “Reread” and “output diffuse”. Set MC cycles to 100. Set both X’s shift width and Q’s shift width to 0.2. Click “generate ZMC input file” and then “run ZMC”.
17. Now run Diffuse from the “Diffuse control panel”. Once the diffuse image has finished calculating view the image using the same cutoffs. If you did everything correctly You should see the below image. Notice how the MC simulation has reduced the intensity of the intermodulation satellites. Try see what happens when rereading the crystal model into ZMC and running another 100 MC cycles.



If you got this far - well done. You’ve probably realized by now your doing some pretty cool stuff with respect to the study of crystals and hopefully it hasn’t been all too difficult. :0.