Interactive Python Programs for Crystallography

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My textbook, Foundations of Crystallography[1] uses MATLAB. Because this is expensive, many of my readers have asked me to use an open source language. The third edition, under preparation, includes many interactive Python crystallography programs.

Eight of these programs will be made available to attendees at this conference along with oral explanations on how to run the programs.

Program 1 introduces Python and creates a two-dimensional oblique unit cell and a three-dimensional triclinic cell. Program 2 populates an oblique unit cell of hexamethylbenzene from the fractional coordinates. Program 3 calculates a point group Cayley (or multiplication) table. Program 4 produces a three-dimensional populated unit cell and its projections calculated from crystallographic parameters found in an external database. Program 5 produces the reciprocal cell superimposed on the direct cell using the G and G* matrices. The input is the unit cell parameters a, b, c, α, β, γ. The output is a*, b*, c*, α*, β*, γ*, G, G*, V and V*. Program 6 calculates a powder diffraction pattern where d-spacings use G*. Program 7 calculates the atomic scattering curves for multiple atoms using the Cromer-Mann coefficients. Finally, Program 8 calculates the electron density map for hexamethylbenzene.

The first four programs emphasize a holistic approach to the symmetries of point groups and space groups. The last four programs explore experimental crystallography exemplified by the reciprocal lattice, powder diffraction patterns, atomic scattering curves, and finally an electron density map. The calculation of the three-dimensional unit cell is an example of mathematical modelling. The information put into the model is the crystal parameters and space group symmetries. The verification of the model is the identification of the two-dimensional space group symmetries of three independent projections. In all cases, the programs are simple, transparent, and explicit.

References

[1] Julian, Maureen M. Foundations of Crystallography with Computer Applications, 2nd edition, CRC Press: New York (2015), ISBN: 978-1466552913.