Notes from the Chat on May 21, 2020

The American Crystallographic Association website: https://www.amercrystalassn.org/

Further resources for FT and structure factors: The second book here https://xray.chem.wisc.edu/recommended-textbooks-on-crystallography/ by Girolami is my favorite. The explanations are very clear. The appendices there will also refresh your math - dot and cross products, complex numbers, etc.

electron density maps are generated in Olex2: Tools > Maps

Q. Do you suffer from additional peaks from fluorescence (when there is fluorescence)? Or is it just heightened background intensity everywhere? A. Heightened background and increased absorption.

Epicycles: https://www.youtube.com/watch?v=QVuU2YCwHjw

Richard Cooper (crystallographer with Crystals program): https://twitter.com/coopallographer

Resources for Crystals: http://www.ccp14.ac.uk/ccp/web-mirrors/crystals/crysworkshop-gettingstarted.html

and

http://www.xtl.ox.ac.uk/crystals/documentation.html

HaRT background:
Jayatilaka & Dittrich., Acta Cryst. 2008, A64, 383

Capelli et al., IUCrJ. 2014, 1, 361

Fugel et al., IUCrJ. 2018, 5, 32
And these are linked from OLEX2: Tools-->HARt

And then, click on "i" next to "HAR Interface"

While I'm going on about HARt, I should mention that you need really, really good data for this to be a reasonable approach.

WinWulff is free; you give it a space group and unit cell, and it will predict a diffraction pattern, but without intensity, because it has not atoms.

You could make CH3CN linear with addition of the 2 1,2 distances set equal to the 1,3 distance