First structures as undergraduate and graduate student

R Castañeda[1]

[1]New Mexico Highlands University

lcast029@uottawa.ca

My first structure was a doped bismuth ferrite perovskite, which was solved in 2012 using Rietveld refinements and performed by the Fullprof software package. Rietveld refinement technique gained rapid popularity and nowadays can be carried out by additional software packages such as TOPAS, GSAS-ii, and Jana, becoming more user-friendly than ten years ago, and resulting in more publications. In the past decade graduate and undergraduate students are solving more single-crystal structures; in part due to Olex2 being a friendly free software with instructional videos on YouTube. My first single-crystal X-ray structures were solved in Olex2, which in my opinion, is the most complete single crystal solution software. Other important changes in recent years worth mentioning are the rise of the pair distribution function (PDF) and the implementation of ShelXT. On the other hand, what has not changed much in the past ten years are sample preparation techniques. The recent advances in solving crystal structures from powder XRD or single-crystal XRD will be presented from the perspective of a recent Ph.D. graduate.