A Tool for Automating the Repetitive Part of PXRD User Reports

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As a service crystallographer in charge of a PXRD instrument, a large part of my job is returning data to the user. Alongside the raw data files, I give a list of the parameters used to gather the data, so the user can include this in a paper if needed. This as-yet-unnamed Python software, greatly reduces the time it takes to type out these parameters each and every time by directly extracting them from the PXRD data files ready to be pasted into a document. This also prevents errors when manually transcribing these parameters. Since the data files were already being parsed, the script also checks for errors a crystallographer can make when setting up a PXRD experiment. Finally, since many of my users are not XRD experts, it exports the data to a CSV file that can be examined in graphing software they are more familiar with.

Accompanying this software is a LaTeX template that takes the output of the Python script and automatically creates a nicely formatted PDF that includes the name and parameters of each experiment alongside a graph of the data.

No knowledge of python or LaTeX is needed to use this software and template.

1 ACA Example

Bragg-Brentano (Coupled θ–θ) Measurement, Incident Slit: 0.681 mm, Step Size: 0.02°, Step Time: 0.25 s, Measurement Range: 35° to 85° 2θ, Total Measurement Time: 11 min.
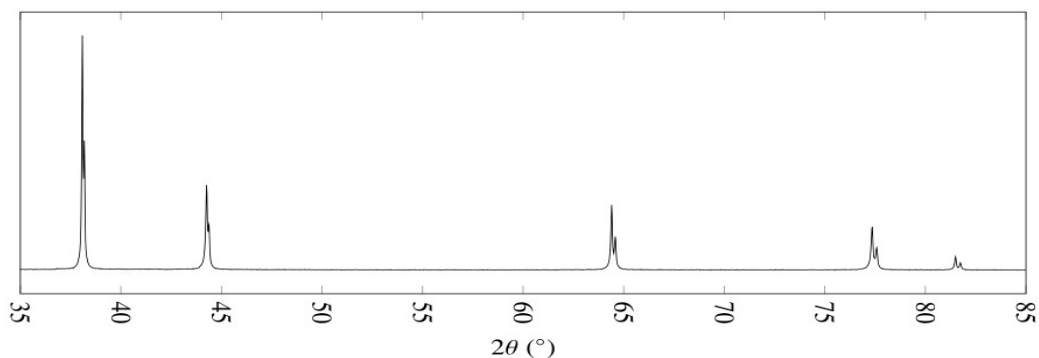

Figure 1: ACA Example