

When Is PXRD Data Good Enough, Or When Should I Stop Trying to Resolve Those Tiny Peaks Out of The Baseline?

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As a service crystallographer with an engineering department, a significant amount of my work involves collecting data for phase identification on samples from industrial processes or dug out of the ground at a work site or similar. These often have many phases and impurities, leading to a significant number of small peaks near the baseline. Extending the duration of the measurement to see these clearly will sometimes unveil more, smaller, peaks. As a service crystallographer, how do you decide when to stop and say “good enough” enough, and when do you tell your user to come back tomorrow because you’re running their sample overnight? How do you prevent every sample from becoming an overnight sample?