# Quantitative crystal structure comparison using powder diffractograms

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Identifying whether two experimental crystal structures determined under different experimental conditions correspond to the same polymorph is a challenging problem in crystallography, with practical (and even legal) implications. We recently developed a new quantitative metric for comparison of powder X-ray diffractograms (PXRD), termed the variable-cell powder difference (VC-PWDF) method. VC-PWDF substantially improves the agreement with COMPACK compared to other PXRD-based comparison tools and is recommended to be used in conjunction with COMPACK to improve reliability of structure comparison. We further extended VC-PWDF to allow direct comparison of both experimental and in-silico-generated crystal structures to collected powder diffractograms. The resulting VC-xPWDF method correctly identified the most similar crystal structure to both moderate and "low" quality experimental powder diffractograms for a set of 7 representative organic compounds, and for the prolific polymorph former, ROY. This approach should allow for rapid identification of new polymorphs from solid-form screening studies by matching to a set of candidates resulting from crystal structure prediction, without requiring single-crystal analysis.

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