

Identification of polymorph type and prediction of materials properties from laboratory x-ray powder patterns using indexing and electron density calculations.

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During routine polymorph or salt screens, x-ray powder measurements are taken of each solid form prepared. Hierarchical cluster analysis (HCA) can be used to automatically group similar patterns together giving a composite pattern of sufficient quality for automated indexing. Derivation of the indexed crystalline unit cell uses knowledge of the starting molecule and its packing ability to restrict the indexing search to only those solutions that allow molecular packing. The derived unit cell can then be used to improve the screening process through a more robust HCA process by matching calculated and measured peak positions. For each new polymorph, the electron density map of the indexed unit cell can be directly derived from structure factors extracted from the composite powder pattern. The resulting electron density distribution allows more reliable prediction of materials properties such as morphology, relative stability and compressibility than knowledge of the crystalline unit cell alone. This allows a ranking of polymorph type according to critical materials properties.