The use of Optical Microscopy and X-ray Powder and Single Crystal Diffraction to Identify and Structurally Characterize Novel Transition Metal Benzoates.

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This research will explore the possibility of replacing medium scale synthesis and crystallization, followed by structural characterization, as a means of discovering new solid-state products, by a series of controlled micro-scale reaction/crystallization experiments using various reagent ratios whilst monitoring changes using microscopy (visible and Raman). By characterizing any crystals that form, the products (monomers, dimers, polymers, clusters, solvates, and polymorphs) can be mapped out in terms of reaction conditions (reagent ratios, solvent, temperature, time in solution).

For example, active pharmaceutical ingredients can be screened for unexpected co-crystal formation when they are mixed with “inactive” ingredients in a formulation. The method could also be used to determine the metal to ligand ratio as well as reaction conditions needed to make novel metal complexes for use as catalysts or as reagents for producing nanomaterials.