

SEMI-AUTOMATION OF STRUCTURE TYPE ASSIGNMENT

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Deriving a starting model is a vital step in any structure refinement method. Structure prototyped Powder Diffraction File entries are beneficial especially when the database does not have the exact chemical composition in search. Keeping this in view, ICDD has editorially prioritized the task to populate the database with structure prototypes. This effort involves identifying possible structure types for about 113,000 inorganic entries. To facilitate this effort, a reference database has been developed housing prime factors that decide the structure type assignment. Several stored procedures have been developed interfacing all the editorial databases to assign the initial structure type. This poster will delineate the process with some case studies.