

Charge Flipping Approach for Inorganic and Organometallic Structures from Powder Data

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Examples of three systems with heavy atom inorganic or organometallic problems will be discussed, and the use of simulated annealing will be compared to charge flipping. Applications of the materials include solid oxide fuel cells, DNA separation adsorbates, and photothermographic film. The simulated annealing approach, both with and without rigid bodies, has been of great value for oxide ceramics, especially for establishing oxygen ion positions in the presence of heavy cations. We demonstrate for several Ba- and Ca-containing silicates that charge flipping is able to find the heavier atoms, but not all of the oxygen ions. Of course, working from the charge flipping solution with Fourier maps is one approach to solving the full structure. In the case of silver organometallics, we show two examples of the use of synchrotron powder data combined with NMR for structure solutions. In one case, successful location of the Ag atoms using charge flipping allows for full structure determination. In the second case, silver Behenate, the structure remains a work in progress.