

Indexing: Algorithms, Accuracy, and *ab initio*

James A. Kaduk

BP Chemicals, P.O. Box 3011 MC F-9, Naperville IL 60566, kadukja@bp.com

Indexing a powder pattern (determining the lattice parameters and symmetry) is a necessary prelude to *ab initio* structure determination and deriving the maximum information from a powder pattern. The different algorithms used by ITO, DICVOL, and TREOR lead to different strategies for their use. The laboratory and synchrotron powder patterns of $(\text{NH}_4)_3(\text{ZnCl}_4)\text{Cl}$ provide an interesting case study of the effects of experimental errors and data processing strategies on the success of indexing. Guaifenesin (3-(2-methoxyphenoxy)-1,2-propanediol), a common expectorant, provides an example of the special problems encountered in indexing the patterns of organic compounds.