

E0006

Polymorph “Prediction”: Where have we been? Where are we now? Where are we going? J. Bernstein, Dept. of Chemistry, Ben-Gurion Univ. of the Negev, Beer Sheva, Israel.

Predict: to see or describe in advance as a result of knowledge, experience, thought, etc.

Acquiring the ability to predict the result of a reaction, the property of a substance or the structure of a material is perhaps the ultimate goal of a chemist since the ability to predict with a high level of confidence implies a corresponding level of understanding and control. Efforts at predicting the crystal structure of a (molecular) substance (or more demanding the structures of expected crystal forms (solvates, salts, cocrystals)) of a (molecular) substance from its structural formula have been continuing for at least half a century, beginning with the pioneering work of Kitaigorodskii. The general lack of success has been noted recently at regular intervals by some leading commentators in the field, in spite of considerable effort and some notable progress. However, for essentially any material it is still not possible to predict the number of crystal forms, their structure, the procedures required to prepare them, or their expected properties.

In this talk we will try to put this area of activity into perspective by reviewing some of those early and current efforts, and suggesting areas of future developments.