Prediction of Zeolite Types Based on Structural Data.[1] M. LACH-HAB, D.A. CARR, I. VAISMAN, E. BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA — Application of knowledge discovery methods in the search of information contained in databases is an emerging field in materials science that plays an important role on facilitating data analysis. In this study we propose a model for identification of the zeolite mineral type based on the topological analysis of the underlying crystal structure. High-throughput generation of topological descriptors is derived from the Delaunay tessellation of zeolite supercells. Based on these descriptors, our Zeolite-Structure-Predictor is trained for classifying zeolite crystals into twenty two different types of minerals and is based on a random forest model constructed with attributes that include tetrahedrality index, in-sphere volume, average edge, frequency of occurrence and probability of oxygen rich selected simplices. The underlying crystal structure data used for this study are included in the Inorganic Crystal Structural Database (ICSD).

Estela Blaisten-Barojas
Computational Materials Science Center,
George Mason University, MS 6A2, Fairfax, VA

Date submitted: 02 Jan 2008   Electronic form version 1.4