A Zeolite Family with Expanding Structural Complexity and Embedded Isoreticular Structures

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The prediction and synthesis of new crystal structures enable the targeted preparation of materials with desired properties. Among porous solid, this has been achieved for metal-organic frameworks, but not for the more widely applicable zeolites, where new materials are usually discovered using exploratory synthesis. Although millions of hypothetical zeolite structures have been proposed, not enough is known about their synthesis mechanism to allow any given structure to be prepared. Here we present an approach that combines structure solution with structure prediction, and inspires the targeted synthesis of new super-complex zeolites. We used electron diffraction to identify a family of related structures and to discover the structural 'coding' within them. This allowed us to determine the complex, and previously unknown, structure of zeolite ZSM-25. By extending our method, we were able to predict other members of a family of increasingly complex, but structurally related, zeolites and to synthesize two more-complex zeolites in the family with much larger cell volumes. Members of this family have the same symmetry, but an expanding unit cell, and are related by hitherto unrecognized structural principles; we call these family members embedded isoreticular zeolite structures.