COMBINATORIAL 2D ZEOLITES

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Abstract

In chemistry, a zeolite is a crystalline solid formed of units consisting of a silicon atom surrounded by four covalently bonded oxygen atoms, see Figure 1. Each

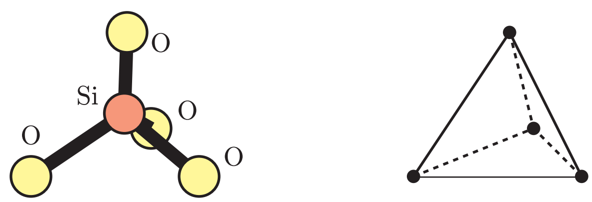

Figure 1. The unit in a zeolite

oxygen has the opportunity to form another bond, but the bond angles in the unit discourage a bond between the oxygens of the same unit as well as more than one bond between oxygens of different units, so it is common for each unit to bonded at the oxygens to four other units. Some zeolites are naturally occurring minerals, others have been synthesized, and still other structures are as yet purely theoretical.

A key feature of zeolites the presence of relatively large empty regions within the solid through which other molecules, such as water or hydrocarbons, may pass, so zeolites are useful in many applications as a micro-filter.

One mathematical model for zeolite structures is to represent each silicon/oxygen unit as a tetrahedron, and to consider arrangements of congruent regular tetrahedra which share corners and do not pairwise interpenetrate. More generally, one can consider analogous abstract mathematical structures both in higher and lower dimensions. For example, if K_3 is the complete graph on three vertices, then the cartesian product $K_3 \times K_3$ is realizable as a unit distance graph in $\mathbb{R}^2$, see Figure 2, which we may regard as a two dimensional combinatorial zeolite.

A *combinatorial d-dimensional zeolite* consists of a connected complex of corner sharing d-simplices such that at each corner there are exactly two distinct simplices, and such that two corner sharing simplices intersect in exactly one vertex. We can conveniently represent a combinatorial zeolite using a *body-pin graph*, whose vertices represent the simplices and whose edges indicate which pair of simplices share a corner. In this case the complex of simplices is simply the line-graph of the body-pin graph. There is a one-to-one correspondence between combinatorial d-dimensional zeolites and d-regular body-pin graphs.

In particular, a 2-dimensional zeolite consists of a complex of triangles two at a vertex, equivalently a 3-regular graph, and a 1-dimensional zeolite is a complex of edges, two at a vertex, in other words, a simple cycle.

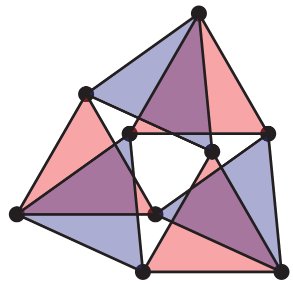

FIGURE 2. $K_3 \times K_3$ as a unit distance graph

By a *realization* of a d-dimensional zeolite we mean an embedding of the d-dimensional complex in $\mathbb{R}^d$, equivalently an embedding of the line graph of the body-pin graph. More chemically relevent is a *unit-distance realization* in which all edges join vertices which are unit distance in $\mathbb{R}^d$, which forces each simplex to be regular.

In this talk we consider the problem of generating examples of combinatorial d-dimensional zeolites and study the dimension of their configuration spaces.

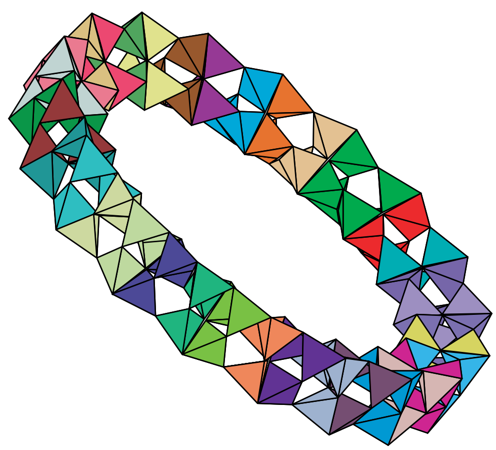

FIGURE 3. A finite 3d zeolite

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