Graph Theoretic Analysis of Zeolite Framework Topologies

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Systematic analysis of zeolite framework topologies (composed of tetrahedral units) can reveal otherwise hidden structural relationships. Sato [1] first showed how unit cells of uninterrupted tetrahedral frameworks can be described as 4-regular 4-connected graphs which contain at least one Hamiltonian cycle. The combinatorial explosion in the number of Hamiltonian cycles and their possible embeddings (drawings) with increasing number of tetrahedral sites, however, has meant that to date only a handful of frameworks have been analyzed directly. Schwalbe-Koda et al. [2] used a graph similarity measure instead and identified several isomorphic topology pairs and triplets. Advances in computational hardware now make it possible to search all possible Hamiltonian cycles and embeddings (drawings) for unit cells with more than 30 T atoms. To perform analyses and compare topologies, however, a method of selecting a canonical form of the Hamiltonian drawing for each framework is needed. Here we report the protocol we developed to achieve this along with results of our analyses.

Zeolite frameworks with up to 38 T atoms in their primitive or conventional unit cells constitute two-thirds of those known to date. We used a conventional backtracking algorithm to calculate all nonequivalent Hamiltonian cycles for these tetrahedral networks. Drawings using each cycle were constructed using a modified form of Sato's method [1] and screened to determine the number of geometrically distinct forms. Graph metrics were then used to select a canonical drawing for each network type in a consisten manner using the python code Zeotopy [3].

Frameworks with the highest topological symmetries were found to be SOD, AHT, ATV, CZP and CHA. As well as confirming the isomorphic topologies reported by Schwalbe-Koda et al. [2], we identified six more pairs: ATS–CAN; DAC–EOS; ITW–JRY; DFT–MON; EWO–TON; and EDI–NAB. Unit cells and isomorphic canonical Hamiltonian graph of EDI and NAB are shown in Fig. 1 as an example.

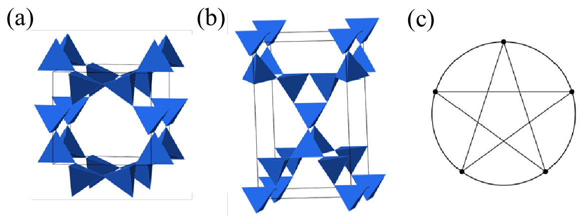

Fig. 1 Primitive unit cells of zeolites (a) EDI and (b) NAB showing SiO_4 tetrahedra, and (c) their shared canonical Hamiltonian graph.

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References

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