Combinatorial aspects of Löwenstein's avoidance rule in aluminosilicates

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According to Löwenstein's rule [1], Al-O-Al bridges are forbidden in the aluminosilicate framework of zeolites. A graph-theoretical interpretation of the rule, based on the concept of independent sets, was proposed earlier [2,3]. It was shown that one can apply the vector method to the associated periodic net and define a maximal Al/(Al+Si) ratio for any aluminosilicate framework following the rule; this ratio was called the independence quotient of the net. The determination of the independence quotient of a periodic net requires finding a subgroup of the translation group of the net for which the quotient graph and a fundamental transversal have the same independence quotient; the respective motif defines a periodic factor of the net. In this talk, I will discuss practical issues regarding the calculation of the independence quotient of mainly 2-periodic nets, with an application to the 200 2-periodic nets listed in the RCSR site [4] and the determination of site distributions realizing this ratio. I will focus on criteria for the choice of the translation subgroup and that of the transversal. In particular, the translation subgroup should be chosen to eliminate every cycle in the quotient graph that is shorter than structural cycles, or rings, of the net. I will show further, that one can take advantage of topological features of the net to define a collection of constraints associated to a maximum independent set and obtain an upper bound for the independence quotient of the net. Active constraints not only provide the value of the independence quotient but in most cases, also the index of the required translation subgroup as well as the nature and number of the different components of the independence factor.

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