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Enumerating Tree Orbits - Application to Viral Capsid Assembly.

Combinatorial methods (permutations, trees, Mobius inversion, generating functions) are used to answer a question about the assembly of icosahedral viral shells. Although the geometric structure of the capsid (shell) is fairly well understood in terms of its constituent subunits (monomers), the assembly process is not. The capsid is modeled by a polyhedron that is a subdivision of the icosahedron and whose facets represent the monomers. The assembly process is modeled by a rooted tree, the leaves representing the facets of the polyhedron, the root representing the assembled polyhedron, and the internal vertices representing intermediate stages of assembly (subsets of facets). To help clarify the effect of symmetry on the probability of the occurrence of a given assembly process a purely combinatorial problem concerning the enumeration of trees is solved. (Received April 04, 2010)