Pólya's Enumeration Theorem Applied to Cubic Unit Cells

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Pólya's Enumeration Theorem utilizes group theory in order to count the number of distinct arrangements of a substituted three-dimensional system based on the fixed points on a shape and its symmetry. This theorem allows calculations of the number of types of unique permutations of substitution sites on a structure without double-counting symmetrically-identical structures. This method has been applied to chemical stereoisomers, but not crystal unit cells. A generating function was created that calculates the number and type of arrangements for simple cubic, body-centered cubic, and face-centered cubic unit cells, based on how many different elements are used in the unit cells. The number of distinct arrangements of elements in these crystal structures has been calculated for the three cubic unit cells. I found that there are 102 ways to arrange an equal amount of two different substituents on a structure with a face-centered cubic unit cell and 554 ways to arrange two different substituents with varying frequencies of substituents. Body-centered cubic, due to having fewer lattice points than the face-centered cubic arrangement, had fewer distinct arrangements per number of substituents. Other amounts of substituents and their implications are discussed.

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