Mathematical Methods in Cluster Science

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Abstract

Nanoclusters are an active research area in many fields of chemistry, physics, materials science, and mathematics. Nanoclusters are created from atoms completing layers or shells sequentially giving rise to what has been phrased as 'magic numbers', or the number of atoms to complete a shell over a beginning layer. Thus, for some clusters, there has developed a large description of formulas, giving the relation of the number of atoms, surface atoms, and bonds as a function of L, the number of shells in the cluster. We describe simple mathematical procedures that apply to nanoclusters and clusters of hypercubes in d-dimensional space to illustrate mathematical properties. Starting with only the atomic coordinates, we create an adjacency and distance matrix that facilitates the calculation of topological indices, including the Wiener, hyper-Wiener, reverse Wiener, Szeged, Balaban, and Kirchhoff indices. Some of the mathematical procedures applied to these structures include: curve fitting (cubics, polynomials, power laws) as it applies to 'magic formulas', topological indices, and functional behavior; interpolation and limits applied to asymptotic behavior of topological indices; composition of functions as applied to topological indices; and logarithms and power laws as applied to informational thermodynamics of nanoclusters. Additionally, we experimentally verify some known topological formulas for hypercubes when $L = 1$. The asymptotic limits with the number of atoms, N, of the topological indices are shown to exhibit power law behavior whose exponent changes with d and type of topological index. The asymptotic graph energy of hypercubes is linear with N, whose slope changes with d, and in 2D agrees numerically with previous calculations. We summarize our calculations with these structures using known mathematical methods.