

Mathematical models for describing molecular self-assembly

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We present several mathematical models for describing molecular building blocks, called rigid tiles, that assemble in larger nanostructures. Rigid tiles can be seen as k -arm branch junction structures that join together by annealing to each other through the affinity of their arm-ends. Such a k -arm rigid tile is described with a set of k vectors joined at the origin that can be translated or rotated during the assembly. Besides the geometric shape of the building blocks, the models can take into account the geometry of the arm-ends joining together. We show distinctions between four models by characterizing types of structures that can be assembled from rigid tiles.