

Boundary effects in the Hexagonal Packing of Rod-like Molecules Inside a Right Circular Cylindrical Domain III. The case of arbitrarily oriented spherocylindrical molecules

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Abstract We study the organization of spherocylindrical molecules inside a freely rotating right circular cylindrical domain at the gas/liquid interface. The analysis is made under the assumption that the molecules are rigid and close packed, and that they are oriented parallel to each other. The direction and angle of their common orientation are completely arbitrary. We obtain exact analytic expressions for the lattice of molecular centers and its boundaries as a function of molecular dimensions, molecular orientation, and domain size. As a first application, we derive the number of molecules in a domain, and the packing fraction. The results obtained are essential when attempting to analytically model a Langmuir film where the global order of the film is less than the local order of the domains.