

Criterion for forming structurally precise nanoparticle by self-assembly

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Multi-subunit proteins and enzymes are well known examples of structurally precise nanoparticles in the size range of 2 to 20 nm. The subunits may be identical as in alcohol dehydrogenase with 4 subunits or they may be different as in hemoglobin with 4 subunits of two kinds, aspartate carbamoyltransferase with 12 subunits of two kinds and G protein with 3 subunits of three kinds. The structural precision of these multi-subunit proteins (viewed here as nanoparticles) is enabled by the unique geometrical shapes of the subunits, the positioning of hydrophobic and hydrophilic regions on the surface, and the availability of hydrogen bonding and salt bridges formation that non-covalently link one subunit to another. Over the last decade, structurally precise aggregates formed from calix(n)arene amphiphiles, also referred to as Platonic micelles, have been reported

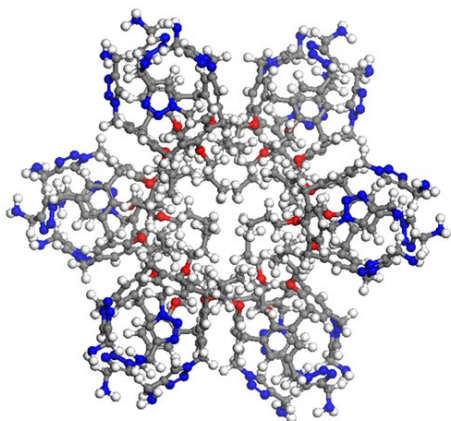


Figure 1: DFT based structure of micelle with aggregation number 6 from PACaL3, a calix[4]arene amphiphile, with primary amine head group and a propyl tail.

in the literature. Their aggregation numbers are discrete, making them analogous to a multi-subunit protein. These aggregates are not stabilized by any non-covalent linkage between the molecules and their formation and stability is driven entirely by hydrophobic effect. Their structural precision, namely, their precise aggregation number is a consequence of how much of the hydrophobic surface of the amphiphile remains exposed to water when they self-assemble into aggregates. In this work, we explore how general this phenomenon of forming structurally precise amphiphilic aggregates can be, starting from common amphiphiles. The analysis of self-assembly of multi-tail amphiphiles each possessing multiple charges shows that by using the criterion of molecular packing and hydrophobic effect, structurally precise amphiphilic aggregates can be generally created via self-assembly.

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