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VIRUS CAPSID MODELING: COMPLEX SELF-ASSEMBLY FROM SIMPLE BUILDING BLOCKS

We present what we believe is the simplest and most versatile virus capsid model to date. Clusters of rigid building blocks composed of one ellipsoid and two 'polarised' repulsive sites can self-assemble not only into shells of icosahedral or octahedral symmetries, but into elongated, 'squashed' shells and double-shell structures as well. The parameter space of the model is very large, with large sections of it favouring particular morphologies (shells, tubes, spirals). For example, when increasing the side-by-side interaction strength between the oblate ellipsoids, we observe the formation of kinetic traps corresponding to competing tubular structures with different radii, analogous to carbon nanotubes with different chirality. Similar structures have been observed *in vitro* for HIV CA proteins. We find single transition state rearrangements during which more strained tubes can relax into less strained morphologies (sliding mechanisms). Other morphologies that self-assemble by simply changing the building block parameters are: capped rods, spirals analogous to tobacco mosaic virus, and even head-tail structures.