Inside the directory "Molecules" are included the cartesian coordinate (XYZ) of all the molecules investigated in this work, including the three hypothetical structures described in the Discussion section. In the directory "Topologies" are the files generated in the group, reporting all the topologies described. The topologies are hand drawn and generated in *pdb* format, and they were created to provide an idea of the underlying topology a molecular assembly may take. Different atoms have been used to colour precursors of different topicity, but the choice of a particular atom does not have any chemical meaning.

Inside each main folder, both molecules and topologies are sorted by family name, as described in the main text.