

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Understanding the self-assembly of meso-tetra(4-sulfonatophenyl)porphyrin (H_2TPPS^{4-}) in aqueous solutions¹ JAVORIS HOLLINGSWORTH, ALLISON RICHARD, GRACA VICENTE, PAUL RUSSO, Louisiana State University — The aggregation of *meso*-tetra(4-sulfonatophenyl)porphyrin (H_2TPPS^{4-}) in phosphate solutions was investigated as a function of pH, concentration, time, ionic strength, and solution preparation (either from dilution of a freshly prepared 2 mM stock or by direct preparation of μM solution concentrations) using a combination of complementary analytical techniques. UV-Vis and fluorescence spectroscopy indicated the formation of staggered, side-by-side (J-type) assemblies. Their size and self-associative behavior was determined using analytical ultracentrifugation and small angle X-ray scattering. Our results indicate that in neutral and basic solutions of H_2TPPS^{4-} , porphyrin dimers and trimers are formed at μM concentrations and in the absence of NaCl to screen any ionic interactions. At these low concentrations and pH 4, the protonated H_4TPPS^{2-} species self-assembles leading to the formation of particularly stable aggregates bearing 25 ± 3 macrocycles. At higher concentrations, these structures further organize or re-organize into tubular, rod-like shapes of various lengths which were imaged by cryogenic and freeze-fracture transmission electron microscopy. Micron-scale fibrillar aggregates were obtained even at μM concentrations at pH 4 when prepared from dilution of a 2 mM stock solution and/or upon addition of NaCl.

¹This research was partially funded by NIH R01 CA098902 and by NSF DMR-1005707.

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Date submitted: 11 Nov 2011

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