

Supporting Information

Solution Structure of Copper-seamed *C*-alkylpyrogallol[4]arene Nanocapsules with Varying Chain Lengths

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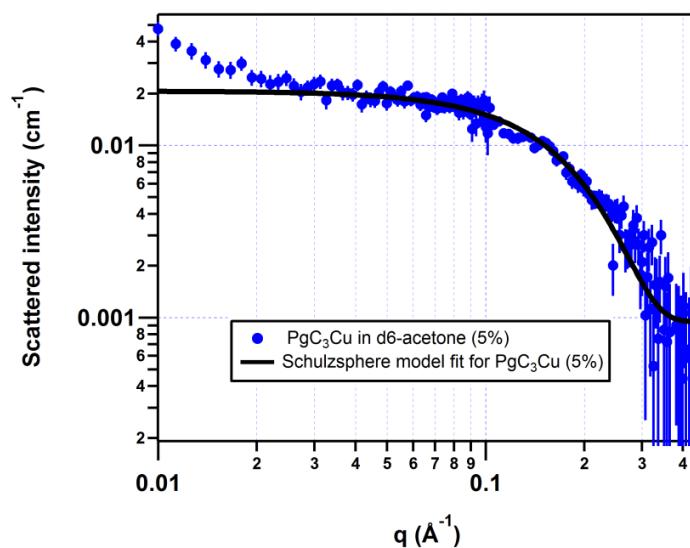
In this section of supporting information, we report the full sets of fitting parameters of the Schulz sphere fit for PgC₃Cu hexamer and global Schulz sphere fits (mass fractions of 1% and 5%) for the PgC₆Cu and PgC₉Cu hexamers. Fitted values reported as (global) are common to both concentrations. Other parameters are local to the listed data set. All uncertainties reported are one standard deviation of that fitted parameter.

Scattering length densities (SLD):

Sample	Molecular formula	Density	wavelength (Å)	SLD
PgC ₃ Cu hexamer	C ₂₄₀ H ₂₁₆ O ₇₂ Cu ₂₄	1.2	6	1.74E-06
PgC ₆ Cu hexamer	C ₃₁₂ H ₃₆₀ O ₇₂ Cu ₂₄	1.2	6	1.42E-06
PgC ₉ Cu hexamer	C ₃₈₄ H ₅₀₄ O ₇₂ Cu ₂₄	1.2	6	1.18E-06

(1) Schulz sphere fit results for PgC₃Cu hexamer

PgC₃Cu in d6-acetone, mass fraction of 5%

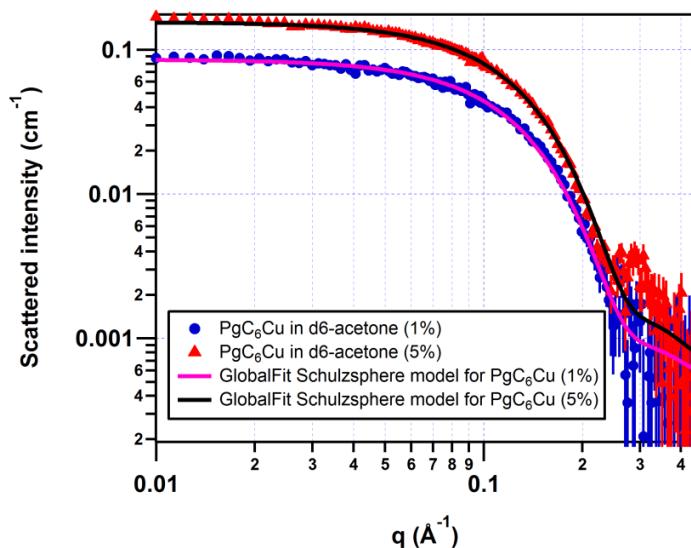


Volume Fraction	0.00198 ± 2.31e-05
Mean radius (Å)	11.12 ± 0.017
Polydispersity (σ_r/r)	0.15 ± 0.00015
SLD sphere (Å ⁻²)	1.74e-06 (held fixed)
SLD solvent (Å ⁻²)	5.39e-06 (held fixed)
bkg (cm ⁻¹ sr ⁻¹)	0.000854 ± 8.92e-05

$$\text{Sqrt}(X^2/N) = 1.42$$

Fitted range = [0,173] = 0.009974 < Q < 0.4385

(2) Global polydisperse Schulz sphere fit results for PgC₆Cu hexamer



Data Set: PgC₆Cu in d6-acetone, mass fraction of 1%

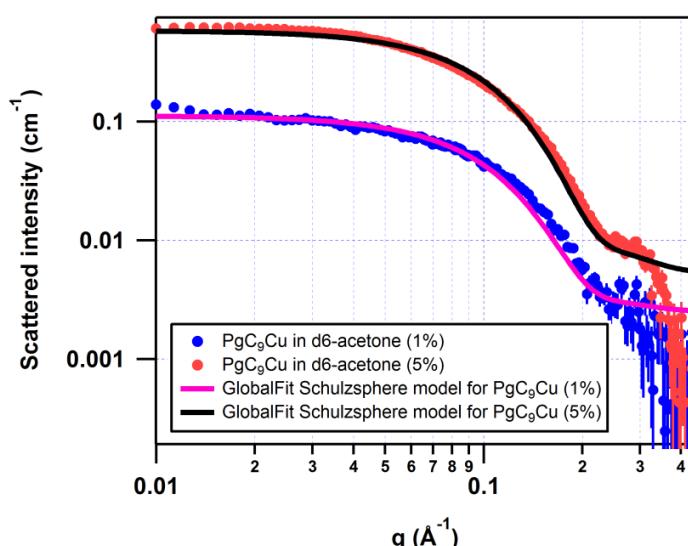
Volume fraction	0.00269 ± 2.38e-05
Mean radius (Å)	14.89 ± 0.15
Polydispersity (σ_r/r)	0.18 ± 0.0067
SLD sphere (Å ⁻²)	1.42e-06 (held fixed)
SLD solvent (Å ⁻²)	5.39e-06 (held fixed)
Bkg (cm ⁻¹ sr ⁻¹)	0.000469 ± 9.09e-05

Data Set: PgC₆Cu in d6-acetone, mass fraction of 5%

Volume fraction (scale)	0.00489 ± 4.01e-05
Mean radius (Å)	14.89 ± 0.15 (global)
Polydispersity (σ_r/r)	0.18 ± 0.0067 (global)
SLD sphere (Å ⁻²)	1.42e-06 (held fixed)
SLD solvent (Å ⁻²)	5.39e-06 (held fixed)
Bkg (cm ⁻¹ sr ⁻¹)	0.000545 ± 0.000105

Sqrt(χ^2/N) 1.29

(3) Global polydisperse Schulz sphere fit results for PgC₉Cu hexamer



Data Set: PgC₉Cu in d6-acetone, mass fraction of 1%

Volume fraction	0.0017 ± 6.48e-06
Mean radius (Å)	17.59 ± 0.015
Polydispersity (σ_z/r)	0.2 (held fixed)
SLD sphere (Å ⁻²)	1.18e-06 (held fixed)
SLD sphere (Å ⁻²)	5.39e-06 (held fixed)
Bkg (cm ⁻¹ sr ⁻¹)	0.00247 ± 8.12e-05

Data Set: PgC₉Cu in d6-acetone, mass fraction of 5%

Volume fraction	0.0092 ± 1.83e-05
Mean radius (Å)	17.59 ± 0.015 (global)
Polydispersity (σ_z/r)	0.2 (held fixed)
SLD sphere (Å ⁻²)	1.18e-06 (held fixed)
SLD sphere (Å ⁻²)	5.39e-06 (held fixed)
Bkg (cm ⁻¹ sr ⁻¹)	0.00506 ± 9.29e-05

Sqrt(χ^2/N)

4.78

NOTE: During the global polydisperse Schulz sphere fit for the PgC₉Cu hexamer at mass fractions of 1% and 5%, the polydispersity was held fixed at 0.2 to ensure that the fitted mean radius is directly comparable to PgC₃Cu and PgC₆Cu.