Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Azaporphine guest-host complexes in solution and gas-phase: evidence for partially filled nanoprisms and exchange reactions

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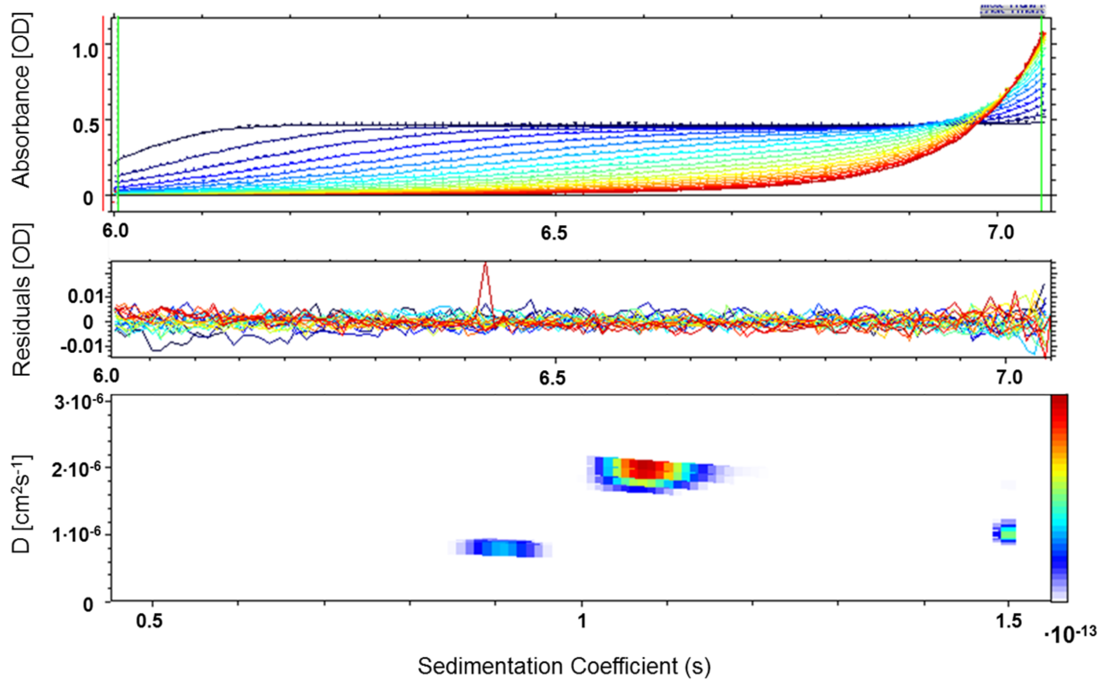
a)



b)

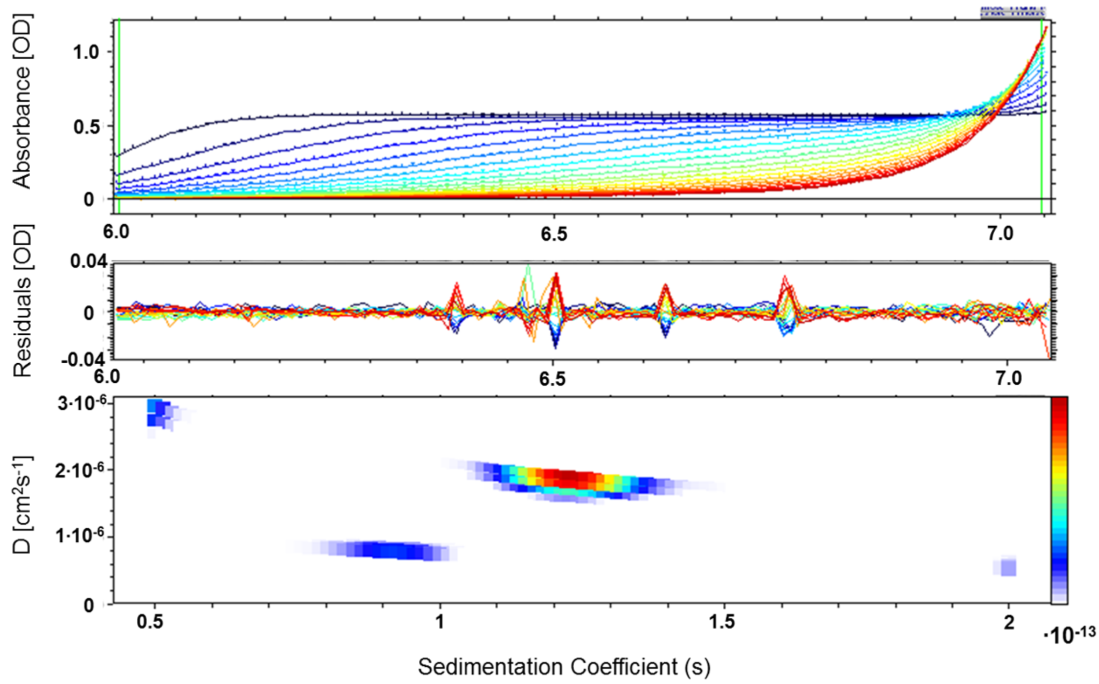


Figure SI 1:
Screenshot of SEDFIT analysis of a) $\mathbf{A}_2\mathbf{B}_3\boldsymbol{H}_3\boldsymbol{Pd}_6(NO_3)_{12}$ and b) $\mathbf{A}_2\mathbf{B}_3\boldsymbol{Cu}_{3-x}\boldsymbol{H}_x\boldsymbol{Pd}_6(NO_3)_{12}$ as measured by AUC at 440 nm.

SI 2:
Data analysis

The size and molar mass of the guest-host complexes were calculated from optimized fits of the SV-AUC data according to the procedure described by Carney et al. in ref. 14 of the main text.

$$\rho_p = \rho_s + 18\eta_s s\left(\frac{1}{D}\frac{k_b T}{3\pi n_s}\right)^{-2}$$

$$M = \frac{s k_b T}{D}\left(1 - \frac{\rho_s}{\rho_p}\right)^{-1}$$

$$d_h = \sqrt{\frac{18\eta_s s}{(\rho_p - \rho_s)}}$$

D - Diffusion constant,
ρ_p - particle (molecule) density,
ρ_s - solvent density,
η_s - solvent viscosity ,
s - sedimentation coefficient,
d_h - hydrodynamic particle diameter
T - temperature

Cu Cage (**A**$_2$**B**$_3$***Cu***$_{3\text{-}x}$***H***$_x$***Pd***$_6$(NO_3)$_{12}$):

D = 2 x 10^{-10} m^2 sec^{-1}
s = 1.2 x 10^{-13} sec
ρ_p = 1471 ± 40 kg m^{-2}
d_h = 2.14 nm
M = 4565 ± 100 Dalton

2H Cage (**A**$_2$**B**$_3$***H***$_3$***Pd***$_6$(NO_3)$_{12}$):

D = 2 x 10^{-10} m^2 sec^{-1}
s = 1.08 x 10^{-13} sec
ρ_p = 1424 ± 15 kg m^{-2}
d_h = 2.14 nm
M = 4419 ± 100 Dalton

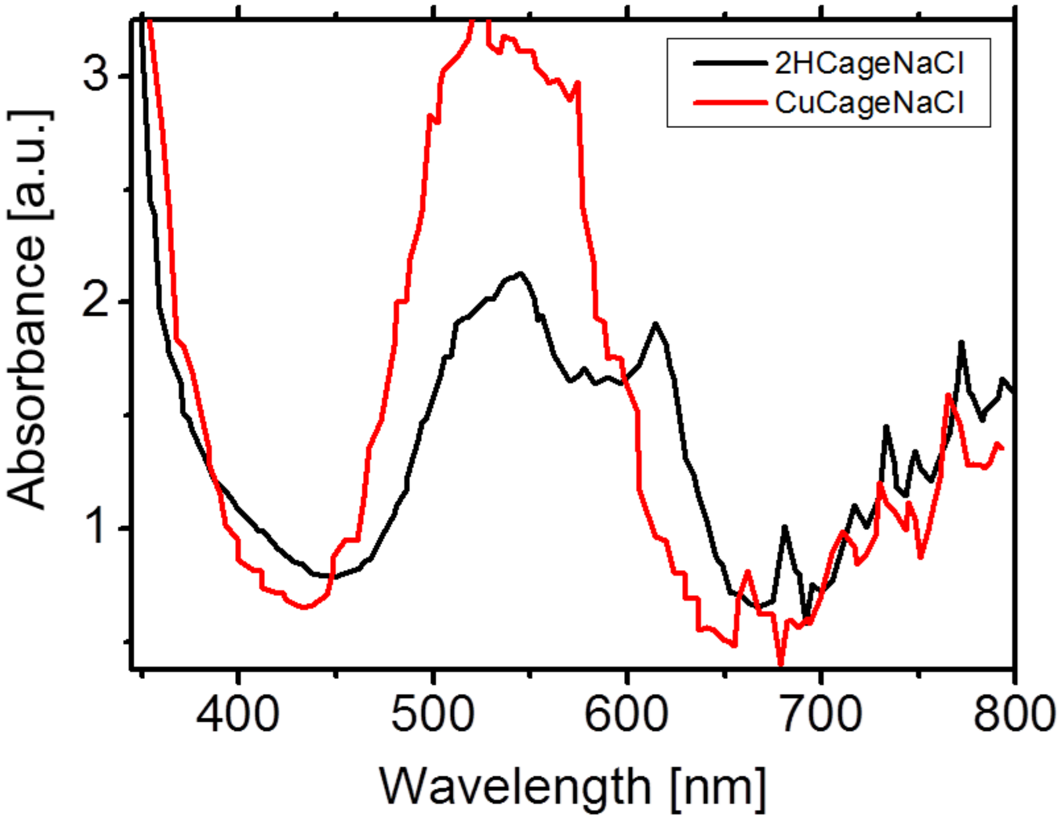


Figure SI 3.
UV vis absorption spectra of
a) Cu Cage ($\mathbf{A}_2\mathbf{B}_3\boldsymbol{Cu}_{3\text{-}x}\boldsymbol{H}_x\boldsymbol{Pd}_6(NO_3)_{12}$, red)
b) 2H Cage ($\mathbf{A}_2\mathbf{B}_3\boldsymbol{H}_3\boldsymbol{Pd}_6(NO_3)_{12}$, black) as measured during AUC at 3000 rpm.

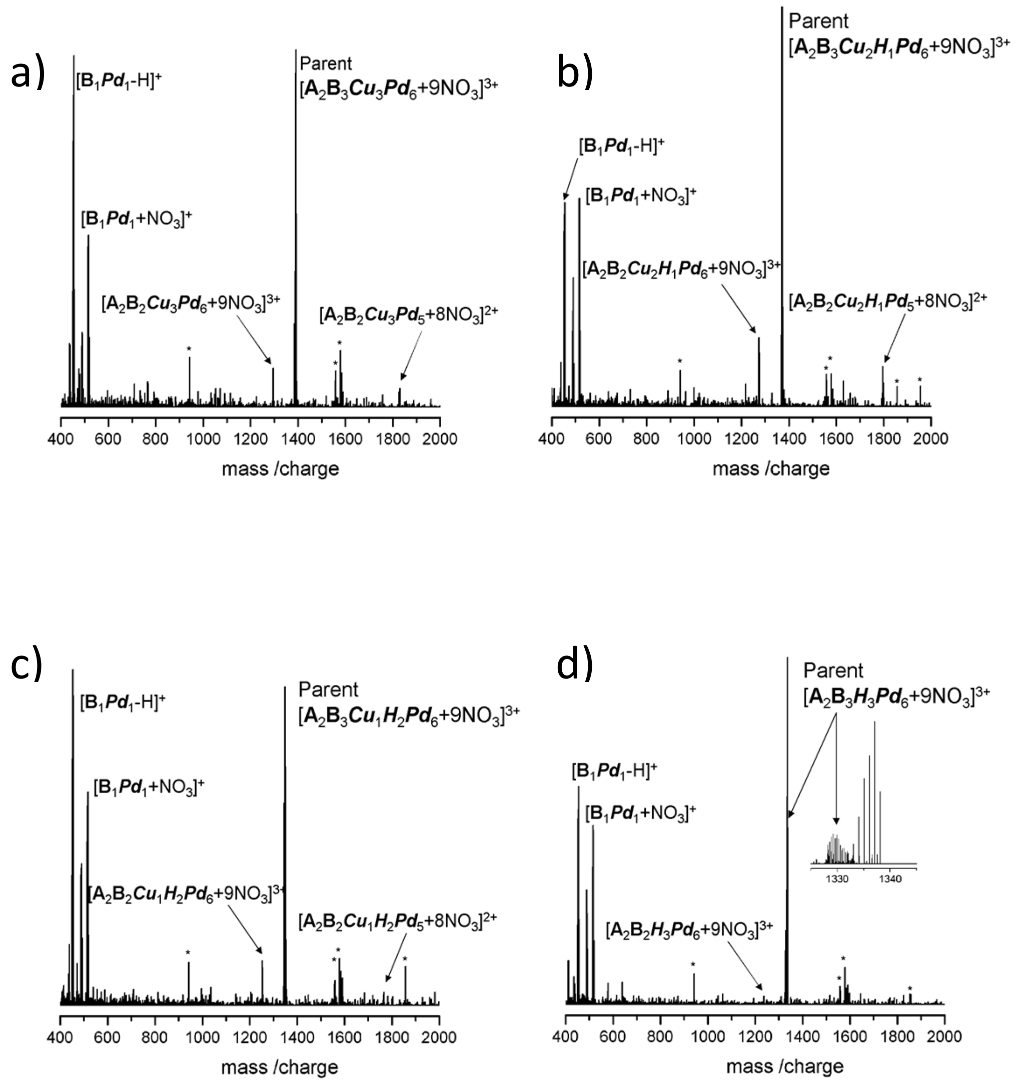


Figure SI 4.
CID mass spectra of [$\mathbf{A}_2\mathbf{B}_3\boldsymbol{Cu}_{3\text{-}x}\boldsymbol{H}_x\boldsymbol{Pd}_6(NO_3)_9]^{3+}$.
a) CID of [$\mathbf{A}_2\mathbf{B}_3\boldsymbol{Cu}_3\boldsymbol{Pd}_6(NO_3)_9]^{3+}$, b) CID of [$\mathbf{A}_2\mathbf{B}_3\boldsymbol{Cu}_2\boldsymbol{H}_1\boldsymbol{Pd}_6(NO_3)_9]^{3+}$, c) CID of [$\mathbf{A}_2\mathbf{B}_3\boldsymbol{Cu}_1\boldsymbol{H}_2\boldsymbol{Pd}_6(NO_3)_9]^{3+}$, d) CID of [$\mathbf{A}_2\mathbf{B}_3\boldsymbol{H}_3\boldsymbol{Pd}_6(NO_3)_9]^{3+}$.The peaks marked by (*) are artefacts and correspond to electronic noise. Isolation width 10 amu, excitation 5 internal units. The dominant fragment is [$\mathbf{B}_1\boldsymbol{Pd}_1$-H]$^+$ in the low mass range, in the high mass range [$\mathbf{A}_2\mathbf{B}_2\boldsymbol{Cu}_{3\text{-}x}\boldsymbol{H}_x\boldsymbol{Pd}_6(NO_3)_9]^{3+}$ is dominating, corresponding the loss of a neutral bipyridine “pillar” **B**.