

Supporting Information

Bridged-Cyclodextrin Supramolecular Hydrogels: Host-Guest Interaction Between Cyclodextrin Dimer and Adamantyl Substituted Poly(acrylate)s

Jie Wang¹, Yisheng Xu^{1*}, Yiming Wang², Jianjia Liu², Jun Xu², Li Li², Hanh-Trang Nguyen³,
Duc-Truc Pham³, Stephen F. Lincoln³, Xuhong Guo^{2*}

¹Shanghai Key Laboratory of Multiphase Materials Chemical Engineering, East China University of Science and Technology, Shanghai 200237, China

²State Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai 200237, China

³School of Chemistry and Physics, University of Adelaide, Adelaide, SA 5005, Australia

*To whom correspondence should be addressed. E-mail: yshxu@ecust.edu.cn (Yisheng Xu),
guoxuhong@ecust.edu.cn (Xuhong Guo)

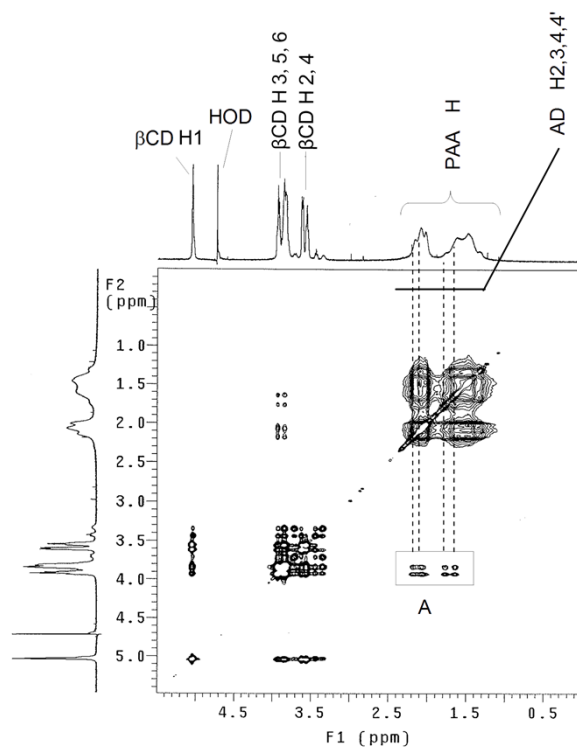


Figure S1. 2D ^1H NOESY NMR spectrum of PAAAD and $\beta\text{CD}_2\text{ur}$ with equimolar βCD groups and adamantyl substituents. The cross-peaks enclosed in rectangle A arise from interactions of the AD substituent H^{2-4} with the annular $\text{H}^{3,5,6}$ of $\beta\text{CD}_2\text{ur}$.

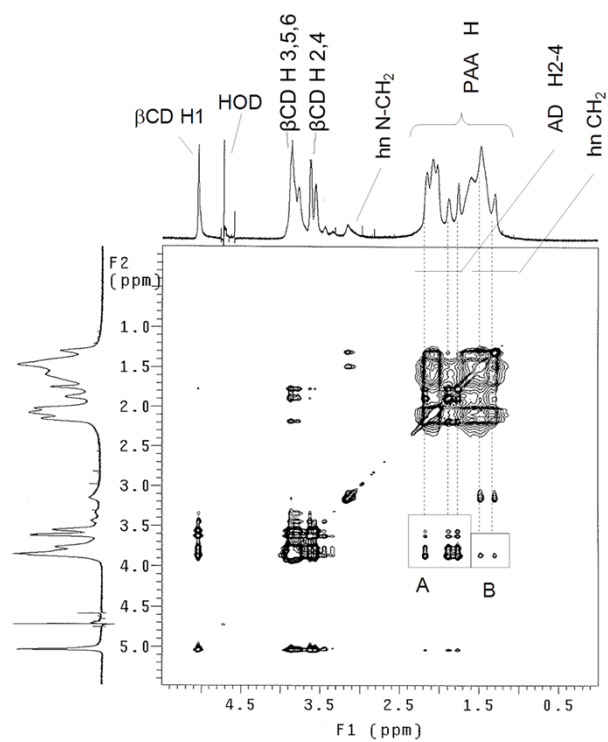


Figure S2. 2D ^1H NOESY NMR spectrum of PAAADhn and $\beta\text{CD}_2\text{ur}$ with equimolar βCD groups and adamantyl substituents. The cross-peaks enclosed in rectangles A and B arise from interactions of the AD substituent H^{2-4} and hexyl tether protons with the annular $\text{H}^{3,5,6}$ of $\beta\text{CD}_2\text{ur}$, respectively.

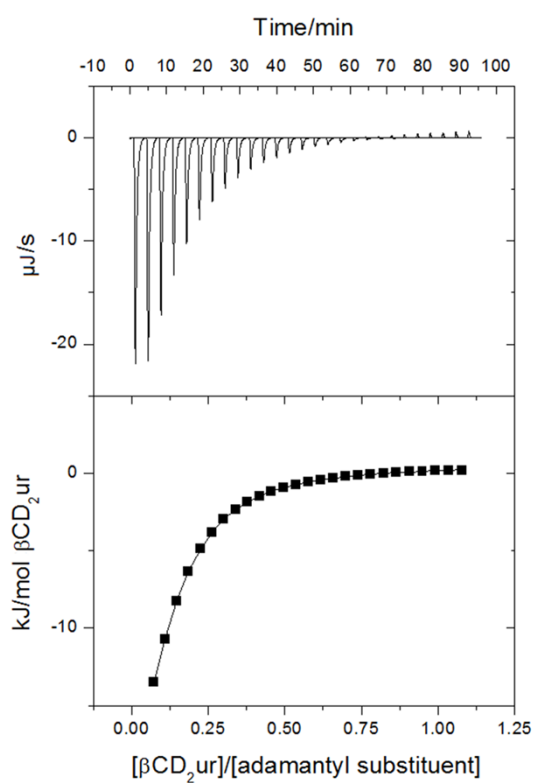


Figure S3. Top. ITC data for the $\beta\text{CD}_2\text{ur}$ /PAAAD system where $6.54 \times 10^{-3} \text{ mol dm}^{-3}$ $\beta\text{CD}_2\text{ur}$ was titrated into 0.4 wt. % PAAAD for which the $[\text{adamantyl substituent}] = 1.22 \times 10^{-3} \text{ mol dm}^{-3}$ in aqueous phosphate buffer at pH 7.0 and $I = 0.10 \text{ mol dm}^{-3}$ at 298.2 K. Bottom. The solid curve shows the best fit to the experimental data points of an algorithm for equilibrium analogous for the interaction of the βCD with the adamantyl substituent.

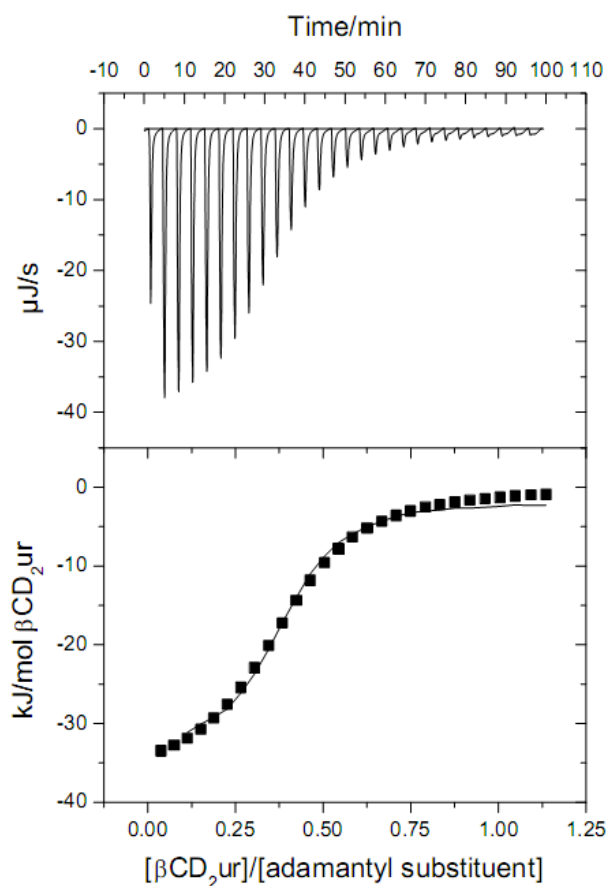


Figure S4. Top. ITC data for the $\beta\text{CD}_2\text{ur}$ /PAAADddn system where $3.27 \times 10^{-3} \text{ mol dm}^{-3}$ $\beta\text{CD}_2\text{ur}$ was titrated into 0.2 wt. % PAAADddn for which the $[\text{adamantyl substituent}] = 0.59 \times 10^{-3} \text{ mol dm}^{-3}$ in aqueous phosphate buffer at pH 7.0 and $I = 0.10 \text{ mol dm}^{-3}$ at 298.2 K. Bottom. The solid curve shows the best fit to the experimental data points of an algorithm for equilibrium analogous for the interaction of the βCD with the adamantyl substituent.