Supporting Information

for

Dynamic light scattering studies of the effects of salts on the diffusivity of cationic and anionic cavitands

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Additional analytical data and NMR spectra

Table of contents

Figure S1: PGSE NMR spectrum of 1	S2	
Figure S2: ¹ H NMR titration of 1 with NaOH	S3	
Figure S3: ¹ H NMR of 1 with CsCl	S4	

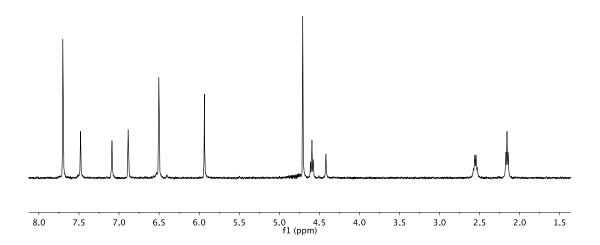


Figure S1: PGSE NMR of 2.00 mM 1 in 20.0 mM NaOH in H_2O .

Compound 1 requires a basic medium to facilitate solubility but is known to aggregate under mildly basic conditions, requiring an increase in pH to ensure monodispersity of the sample. Before performing DLS titrations, a ¹H NMR titration of 1 with NaOH was performed (Figure S2) to determine a suitable range where 1 would be monodisperse but the presence of excess salt would be minimized. The titration revealed that at 10 equiv (20 mM) NaOH (NMR 8 in Figure S2), the host is both fully dissolved and monodisperse. Cations play a muted role in the DLS measurements of this study and that fact, coupled with the highly solvated carboxylates of 1 (see main text) suggest that the presence of additional sodium ions should have a negligible impact on the results. Likewise, the hydroxide was mostly consumed in the deprotonation and solubilization of 1, leaving only trace amounts present in solution. Again, this should have a negligible impact on the DLS results.

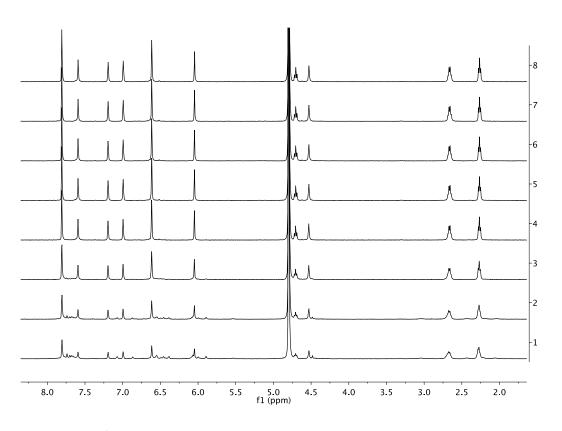


Figure S2: ¹H NMR titration of 1 with 268.0 mM NaOH from 6.5 (NMR 1) to 10 equiv (NMR 8).

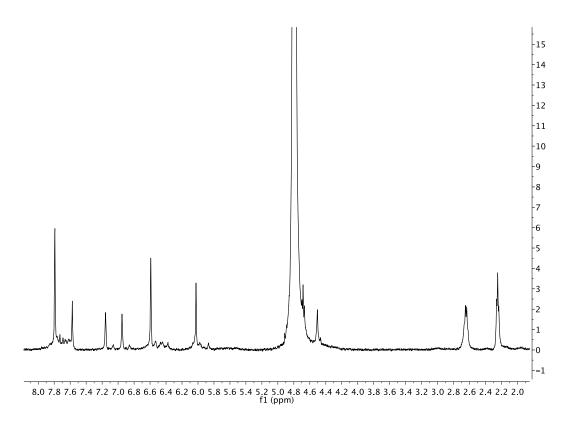


Figure S3: ¹H NMR of 2.0 mM 1 in 20 mM NaOH + 100 mM CsCl.