Supplemental Material

The host-guest complexations of amine boranes and isoelectronic/isostructural quaternary alkylammonium cations by cucurbit[7]uril in aqueous solution

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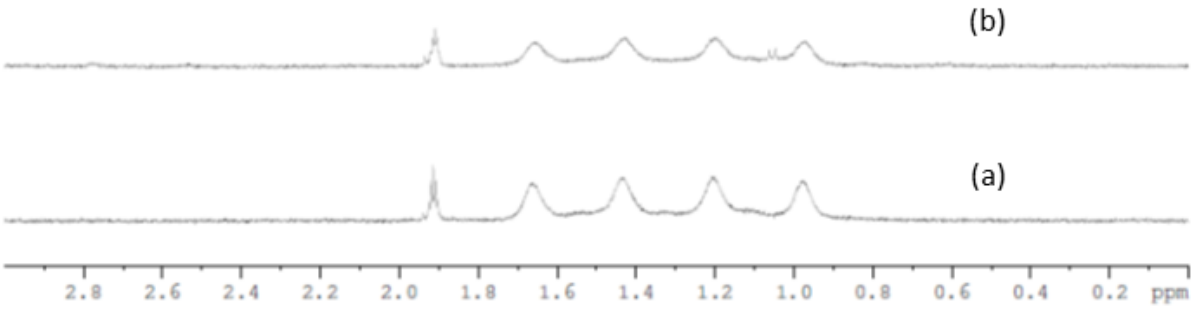

Figure S1. ^{1}H NMR spectra of ammonia borane (1.0 mM) in the (a) absence and (b) presence of CB[7] (2.5 mM) in D_2O (pD = 4.75). Peak at 1.92 ppm is due to the residual protons from the acetate buffer.

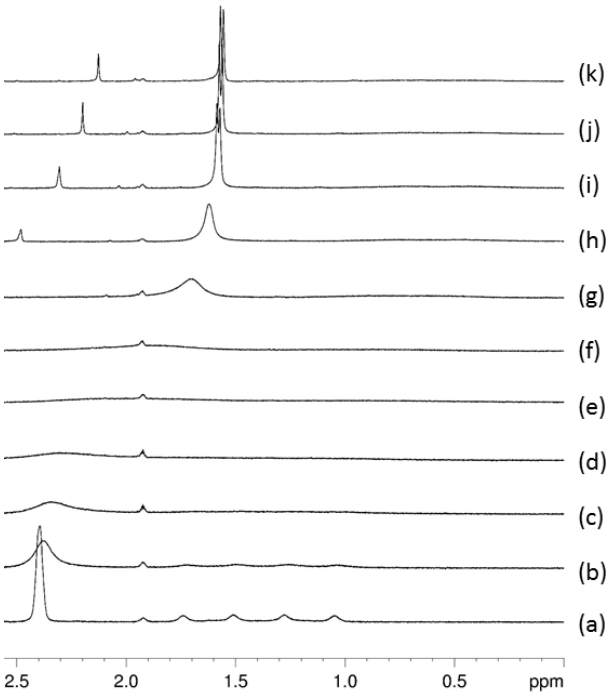

Figure S2. ^{1}H NMR spectra for $(CH_3)_2HNBH_3$ (1.00×10^{-3} M) in the presence of (a) 0.00, (b) 0.17, (c) 0.49, (d) 0.60, (e) 0.88, (f) 1.00, (g) 1.48, (h) 1.60, (i) 2.34, (j) 3.26, and (k) 4.00 equivalents of CB[7] in D_2O. (pD = 4.7)

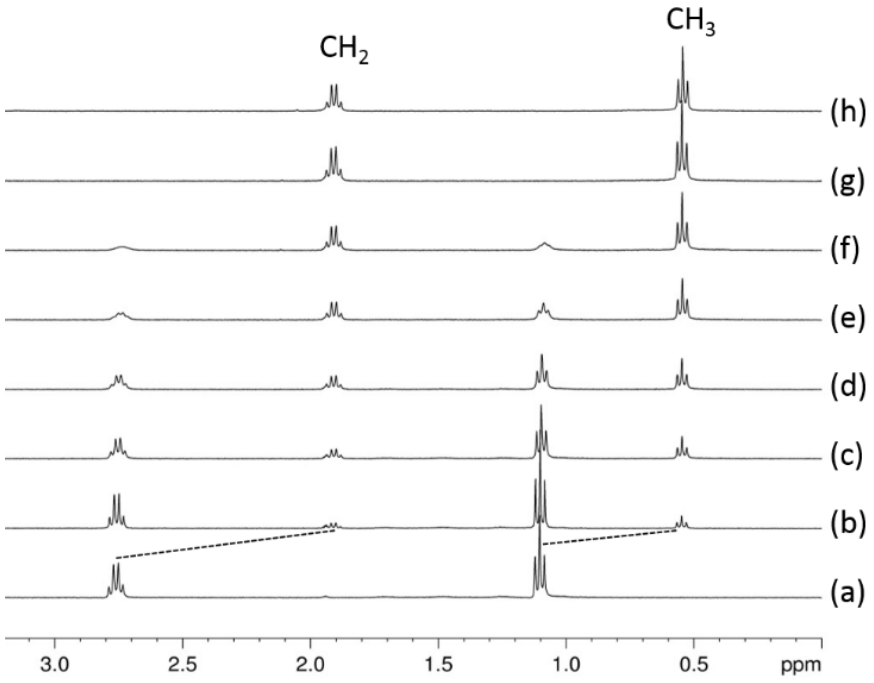

Figure S3. ^{1}H NMR spectra of $(CH_2CH_3)_3NBH_3$ (1.0×10^{-3} M) in the presence of (a) 0.00, (b) 0.16, (c) 0.30, (d) 0.44, (e) 0.62, (f) 0.81, (g) 1.17, and (h) 2.24 equivalents of CB[7] in D_2O (pD = 4.7).

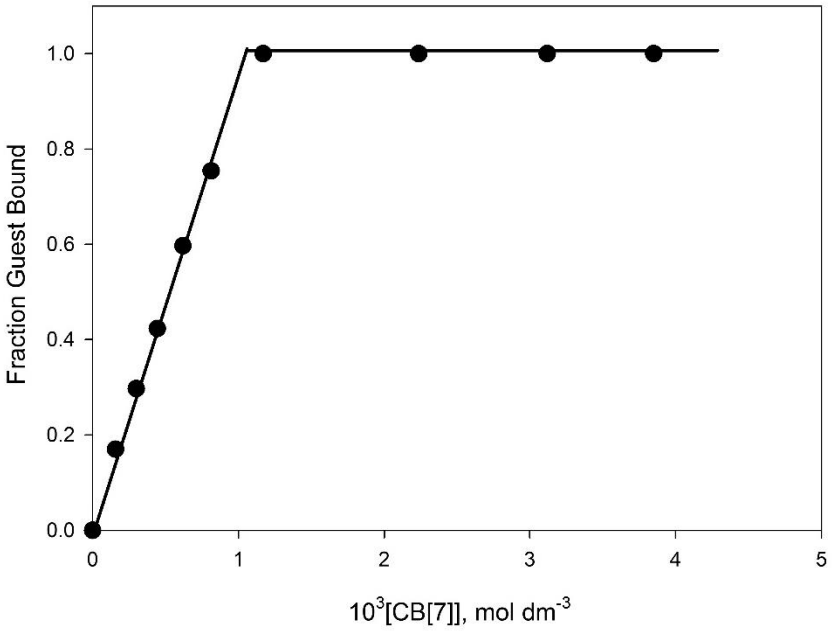

Figure S4. Plot of the chemical shift for the methyl proton resonance of $(CH_2CH_3)_3NBH_3$ (1.00 x 10^{-3} M) as a function of [CB[7]] in D_2O.

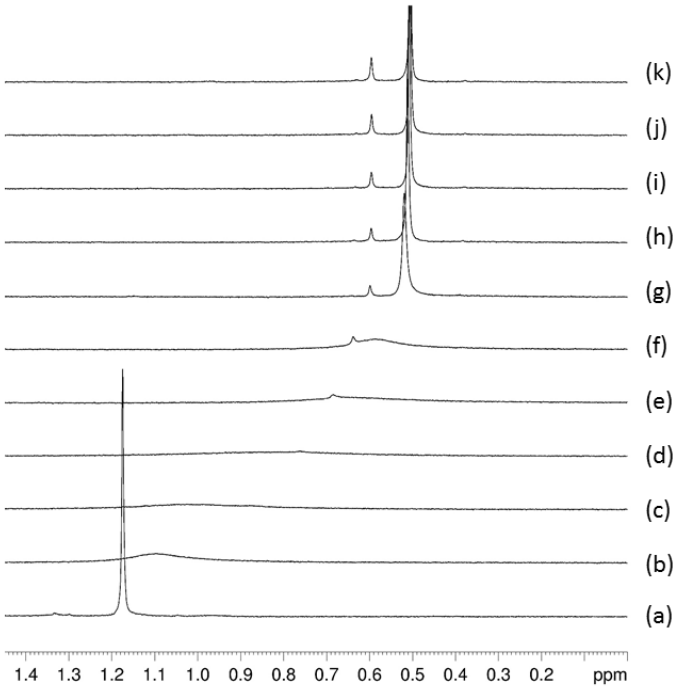

Figure S5. ^1H NMR spectra for $C(CH_3)_3H_2NBH_3$ (1.00 x 10^{-3} M) in the presence of (a) 0.00, (b) 0.18 , (c) 0.32, (d) 0.51, (e) 0.68, (f) 0.86, (g) 1.17, (h) 1.57, (i) 2.51, (j) 3.23, and (k) 4.10 equivalents of CB[7] in D_2O.

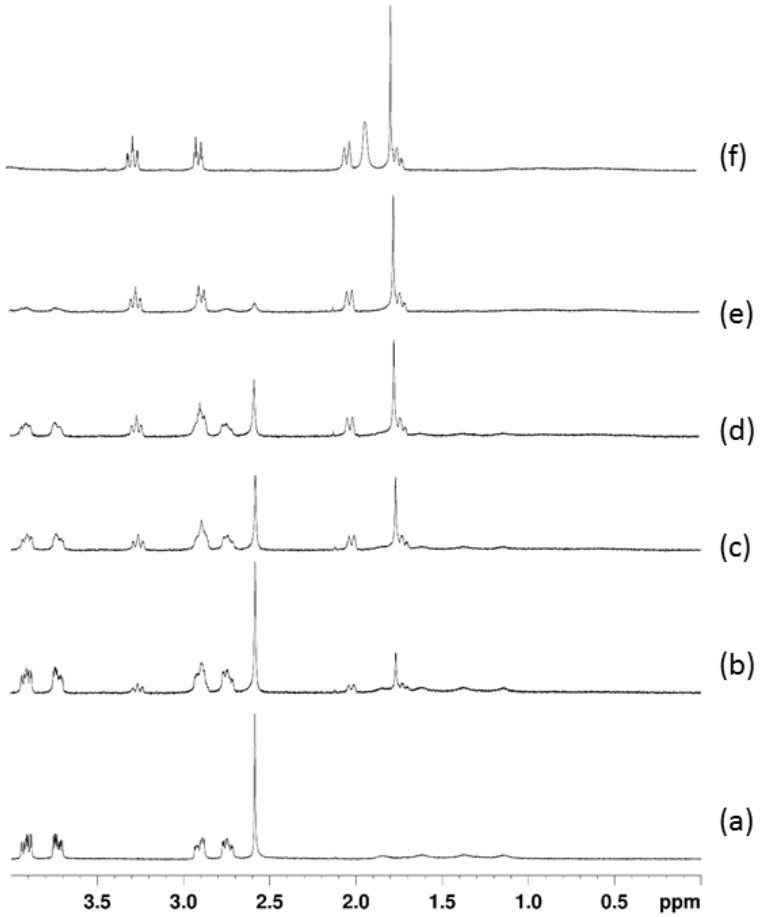

Figure S6. ^{1}H NMR spectra for N-methylmorpholine borane (1.00 x 10^{-3} M) in the presence of (a) 0.00, (b) 0.20, (c) 0.41, (d) 0.62, (e) 0.83, and (f) 1.55 equivalents of CB[7] in D_2O.

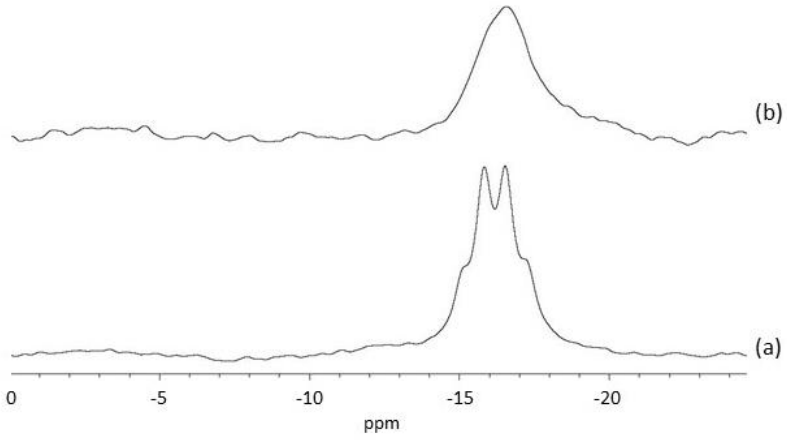

Figure S7. ^{11}B NMR spectra for morpholine borane (1.00 x 10^{-3} M) in the presence of (a) 0.0 and (b) 1.4 equivalents of CB[7] in D_2O.