

Electronic Supplementary Information

Cucurbit[7]uril host-guest complexes and pseudorotaxanes with α,ω -bis(pyridinium)alkane dications

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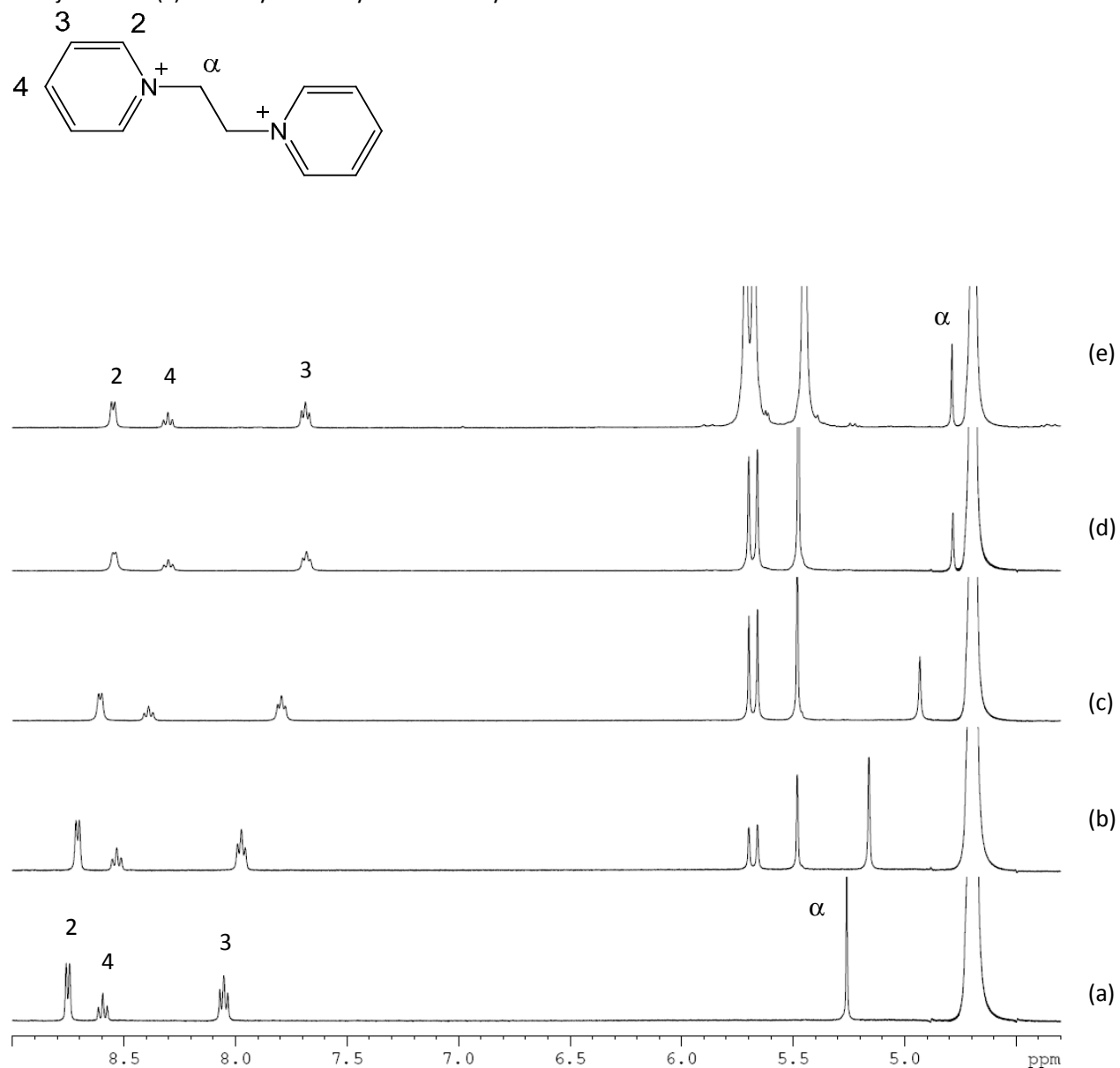


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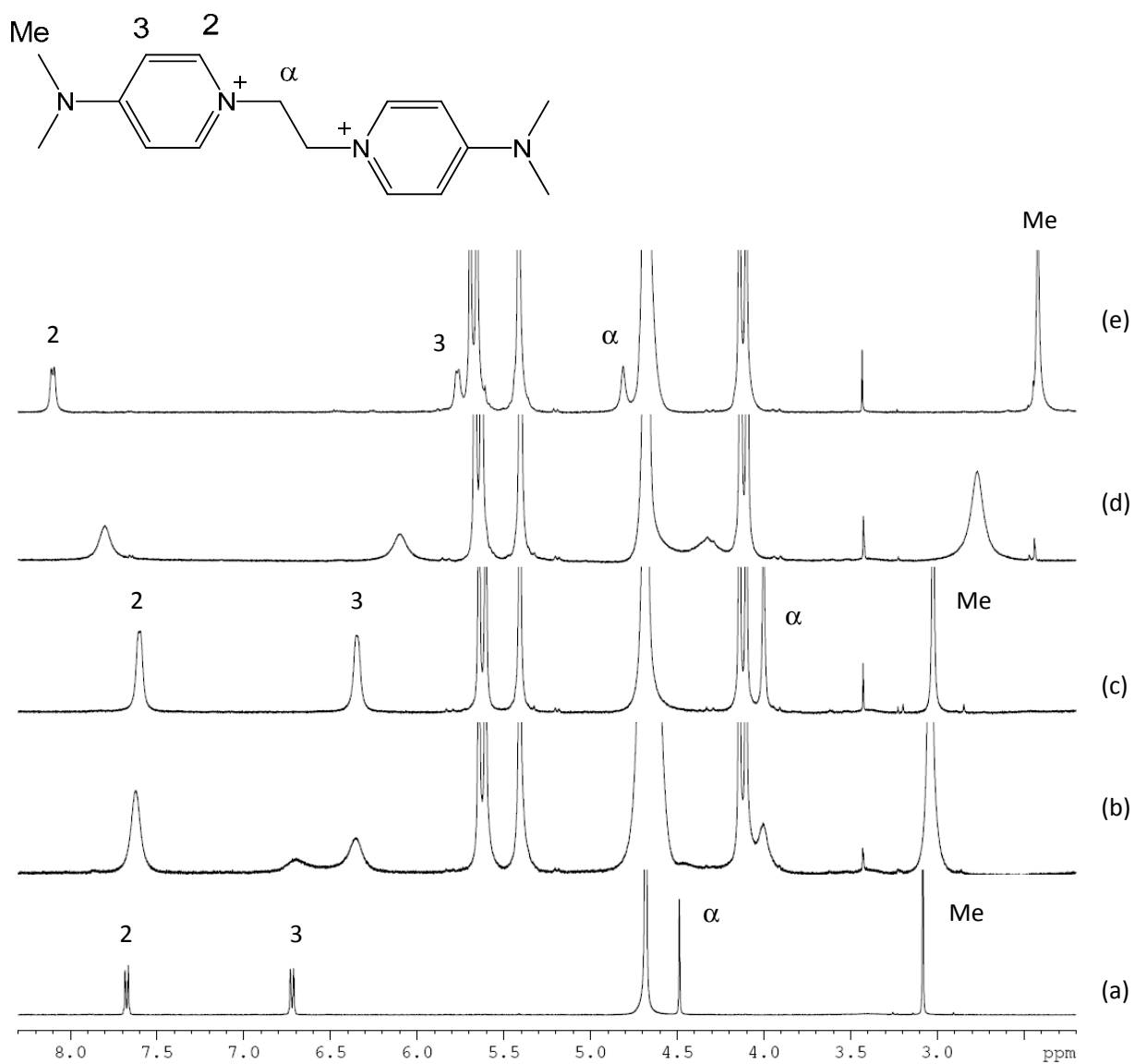


Figure S2. ¹H NMR spectra of BAPE²⁺ ($1.08 \times 10^{-3} \text{ mol dm}^{-3}$) in the presence of (a) 0.00 equiv, (b) 0.73 equiv, (c) 1.14 equiv, (d) 1.86 equiv, and (e) 2.34 equiv of CB[7] in D₂O.

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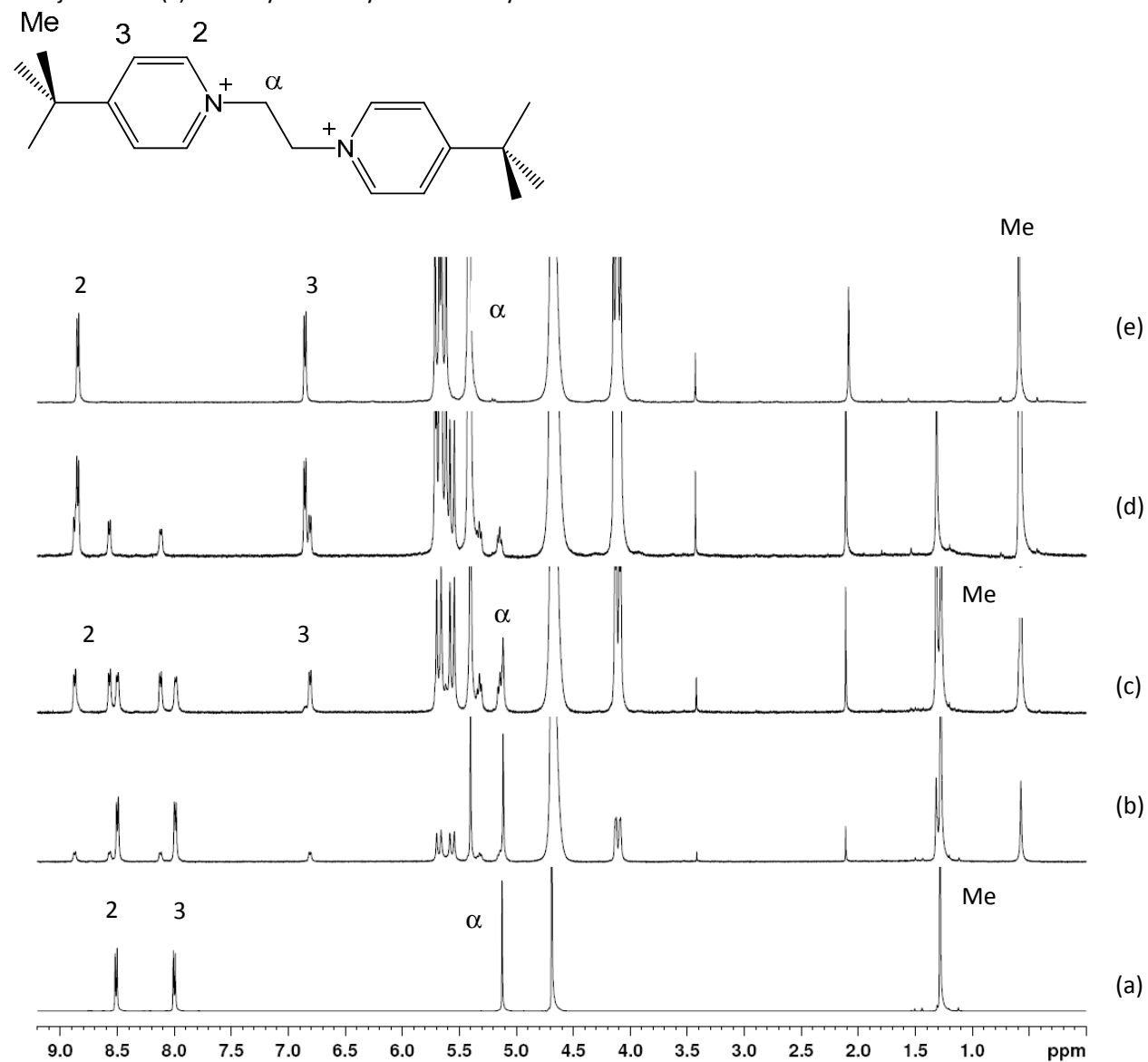


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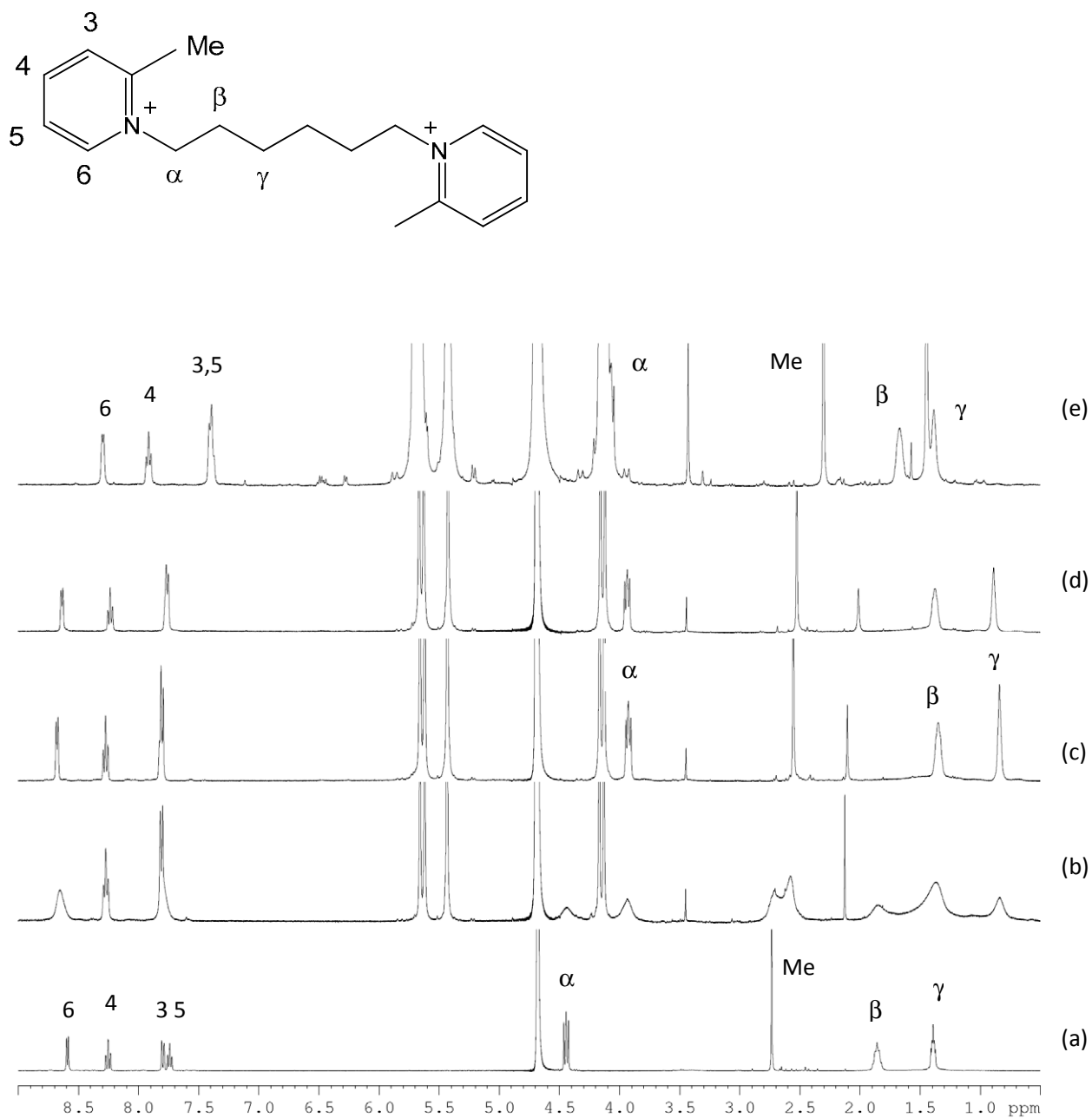


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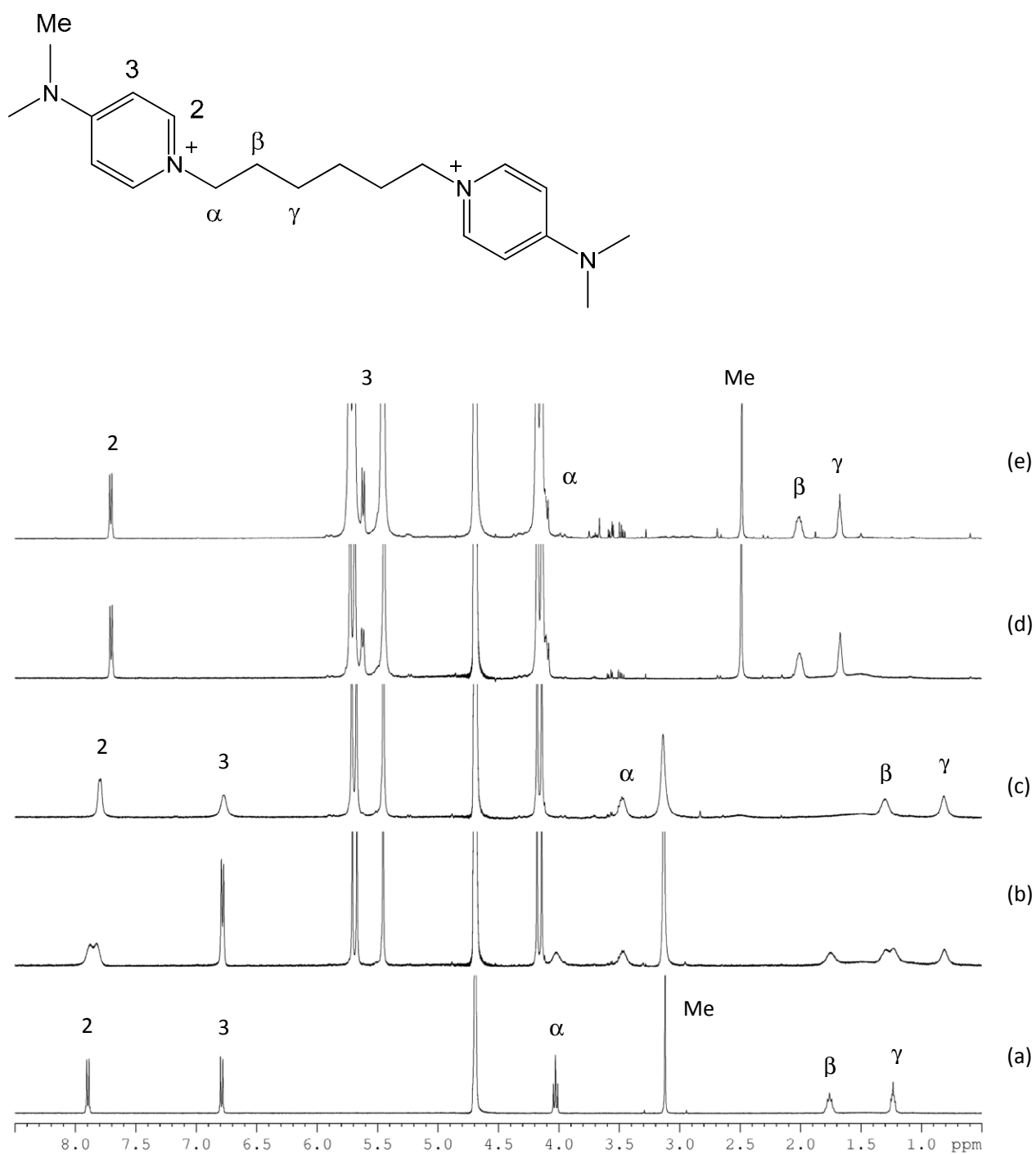


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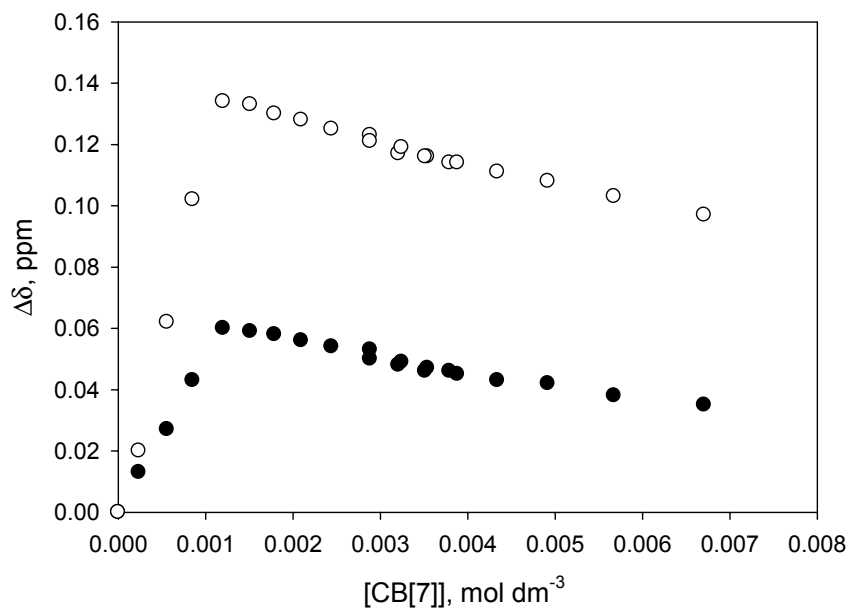


Figure S10. ^1H NMR chemical shift titration of BPH^{2+} ($1.13 \times 10^{-3} \text{ mol dm}^{-3}$) with CB[7] in D_2O . The solid circles are for the H3/H5 protons, while empty circles are for the H4 protons

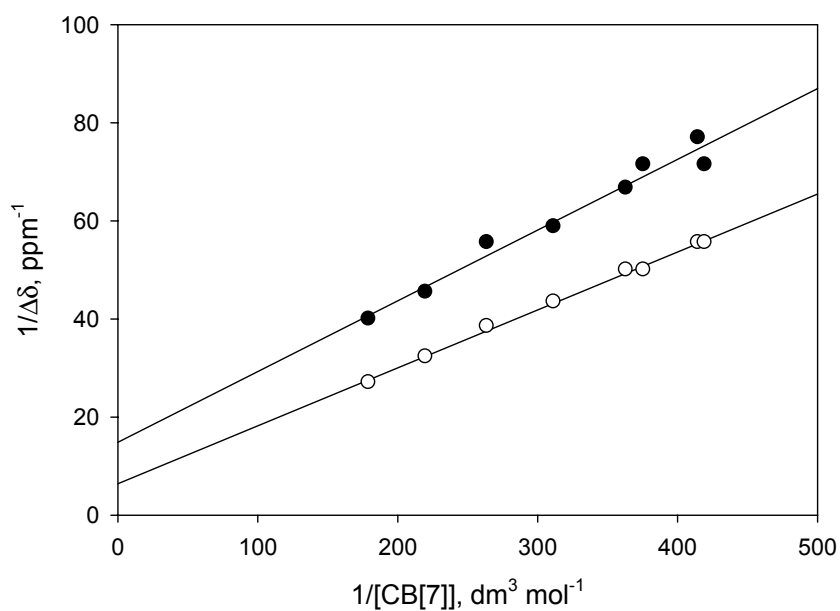


Figure S11. Double reciprocal plot of $1/\Delta\delta$ against $1/[\text{CB}[7]]$ for the titration of BPH^{2+} ($1.13 \times 10^{-3} \text{ mol dm}^{-3}$) with CB[7] in D_2O . The solid circles are for the H3/H5 protons, while empty circles are for the H4 protons

Table S1. Mass spectral peaks for the 1:1 and 2:1 CB[7] host-guest complexes in aqueous solution (calculated values given in parentheses).

Guest	$[M \cdot \text{CB}[7] - 2\text{Br}]^{2+}$	$[M \cdot 2\text{CB}[7] - 2\text{Br}]^{2+}$
BPE ²⁺	674.2286 (674.2291 for C ₅₄ H ₅₆ N ₃₀ O ₁₄ ²⁺)	not observed
BAPE ²⁺	717.2748 (717.2723 for C ₅₈ H ₆₆ N ₃₂ O ₁₄ ²⁺)	1298.4761 (1298.4431 for C ₁₀₄ H ₁₁₆ N ₆₀ O ₂₈ ²⁺)
BBPE ²⁺	730.2947 (730.2927 for C ₆₂ H ₇₂ N ₃₀ O ₁₄ ²⁺)	1311.4967 (1311.4635 for C ₁₀₄ H ₁₁₄ N ₅₈ O ₂₈ ²⁺)*
BPH ²⁺	702.2599 (702.2603 for C ₅₈ H ₆₄ N ₃₀ O ₁₄ ²⁺)	1283.4428 (1283.4321 for C ₁₀₀ H ₁₀₆ N ₅₈ O ₂₈ ²⁺)
B2PH ²⁺	716.40959 (716.2760 for C ₆₀ H ₆₈ N ₃₀ O ₁₄ ²⁺)	1298.2939 (1297.4478 for C ₁₀₂ H ₁₁₀ N ₅₈ O ₂₈ ²⁺)
B3PH ²⁺	716.2784 (716.2760 for C ₆₀ H ₆₈ N ₃₀ O ₁₄ ²⁺)	1297.4906 (1297.4478 for C ₁₀₂ H ₁₁₀ N ₅₈ O ₂₈ ²⁺)
BAPH ²⁺	745.3032 (745.3025 for C ₆₂ H ₇₄ N ₃₂ O ₁₄ ²⁺)	1326.5051 (1326.4743 for C ₁₀₄ H ₁₁₆ N ₆₀ O ₂₈ ²⁺)
BBPH ²⁺	758.3227 (758.3229 for C ₆₆ H ₈₀ N ₃₀ O ₁₄ ²⁺)	1339.5195 (1139.4947 for C ₁₀₈ H ₁₂₂ N ₅₈ O ₂₈ ²⁺)
BBPX ²⁺	768.3064 (768.3131 for C ₆₈ H ₇₆ N ₃₀ O ₁₄ ²⁺)	1349.5275 (1349.4792 for C ₁₁₀ H ₁₁₈ N ₅₈ O ₂₈ ²⁺)

*881.9857 (881.9721 for $[M \cdot 2\text{CB}[7] - 2\text{Br} + \text{Na}]^{3+}$)