Electronic Supplementary Information

Inclusion of Potassium 4,4’-Diphenyldicarboxylate into β-Cyclodextrin: The Design and Synthesis of an Organic Secondary Building Unit

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1 – Synthesis and Structural Characterisation of K$_2$bpdc

1.1 – Synthesis

This compound was used for the preparation of the NMR solutions and for comparison purposes in the vibrational spectroscopy studies. It was prepared as described for the preparation of K$_2$bpdc solution, pH=7.5. A pale green powder was obtained by lyophilisation followed by drying in a desiccator.

Selected FT-IR data (ATR, in cm$^{-1}$): 1581s, 1536s, 1384mbr, 1352sh, 1180w, 1121w, 1097w, 1009w, 837m, 761w, 696m, 677m, 512w, 465w and 394m. No bands were detected above 1600 cm$^{-1}$.

Selected FT-Raman data (in cm$^{-1}$): 3072m, 3046, 1605vs, 1418m, 1281m, 1207w, 1136m, 849m, 824w, 796w, 752w, 628w, 520w, 408w, 329w, 326w and 236.
1.2 – Vibrational Spectroscopy and Theoretical Calculations

1.2.1 – FTIR-ATR

**Figure S1.** Comparison between the experimental (black) FT-IR spectrum of K$_2$bpced and the simulated (red) one for the bpde$^{2-}$ anion. Calculated at B3LYP/6-31G level with the correction factor 0.9627.$^1$
1.2.2–FTIR-Raman

**Figure S2.** Comparison between the experimental (black) FT-Raman spectrum of K₂bpcd and the simulated (red) one for the bpdc⁻² anion. Calculated at the B3LYP/6-31G level with the correction factor 0.9627.¹
2 – Structural Characterization of 1 and 2

2.1 – Thermogravimetric Analysis

Figure S3. TGA of compounds 1 (black) and 2 (red).
2.2 – FTIR-ATR

Figure S4. FT-IR ATR spectra of compounds 1 and 2. The spectra of β-CD and K₂bpdc are also represented for comparative purposes. The two latter spectra were scaled and subject to an offset for clarity purposes.
Figure S5. FT-Raman spectra of compounds 1 and 2. The spectra of β-CD and K₂bpdc are also represented for comparison.
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