Supplementary Material (ESI) for New Journal of Chemistry

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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A contribution from

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Contents

1 – Synthesis and Structural Characterisation of K_2bpdc

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_2bpdc 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

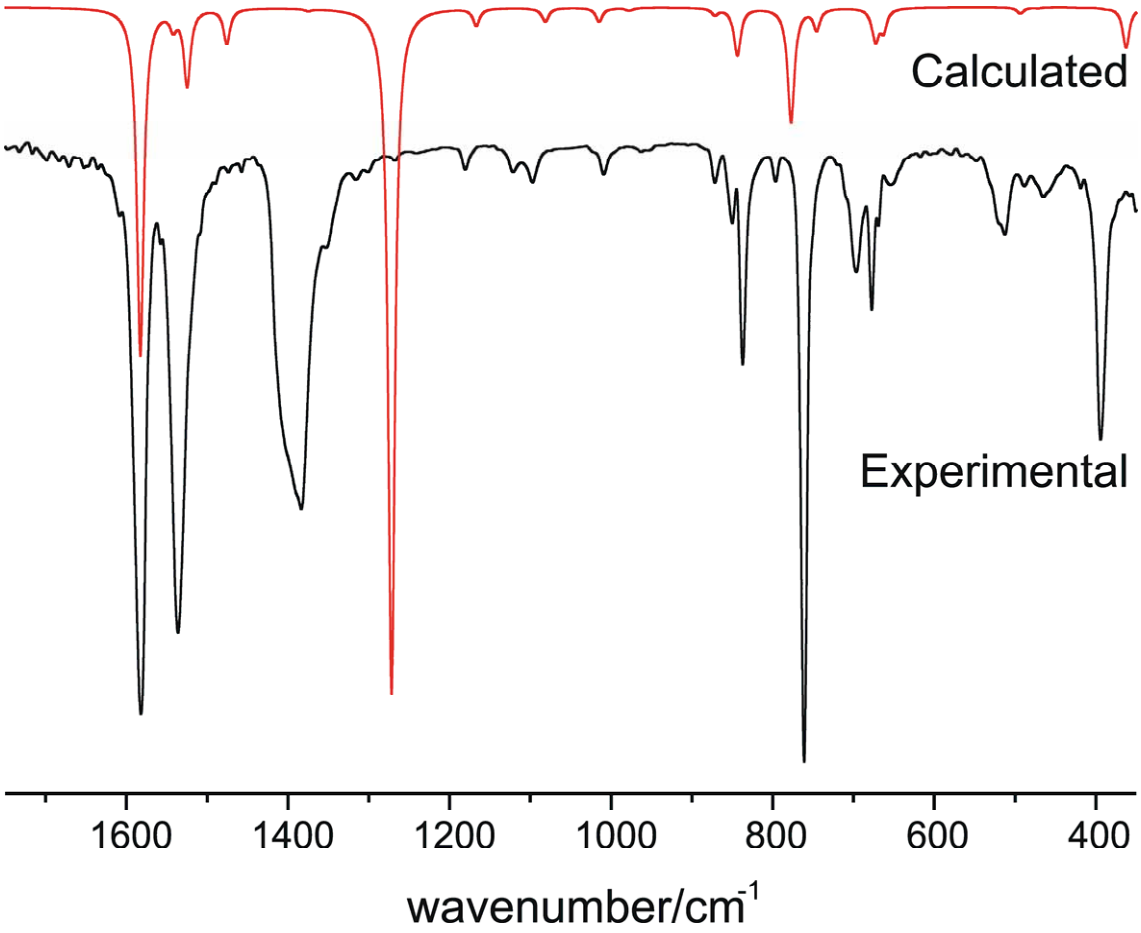

Figure S1. Comparison between the experimental (black) FT-IR spectrum of K_2bpcd and the simulated (red) one for the $bpdc^{2-}$ anion. Calculated at B3LYP/6-31G level with the correction factor 0.9627.[1]

1.2.2–FTIR-Raman

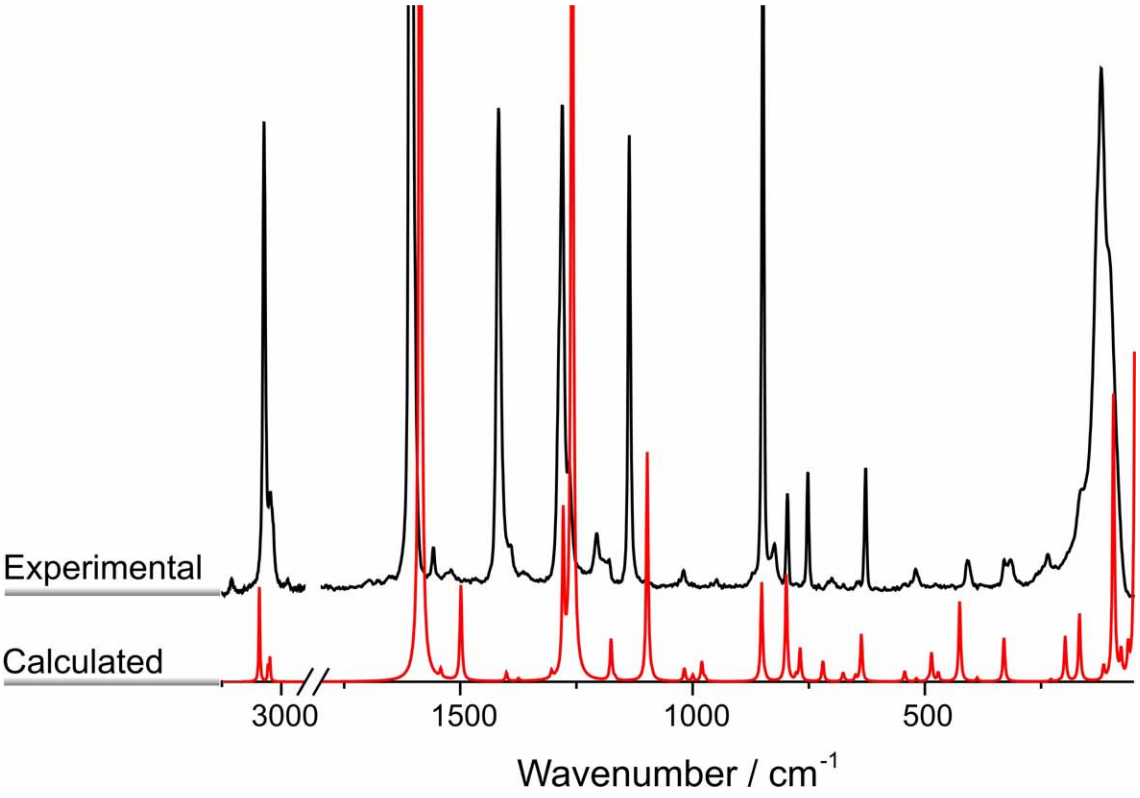

Figure S2. Comparison between the experimental (black) FT-Raman spectrum of K_2bpcd and the simulated (red) one for the $bpdc^{2-}$ anion. Calculated at the B3LYP/6-31G level with the correction factor 0.9627.[1]

2 –Structural Characterization of 1 and 2

2.1 – Thermogravimetric Analysis

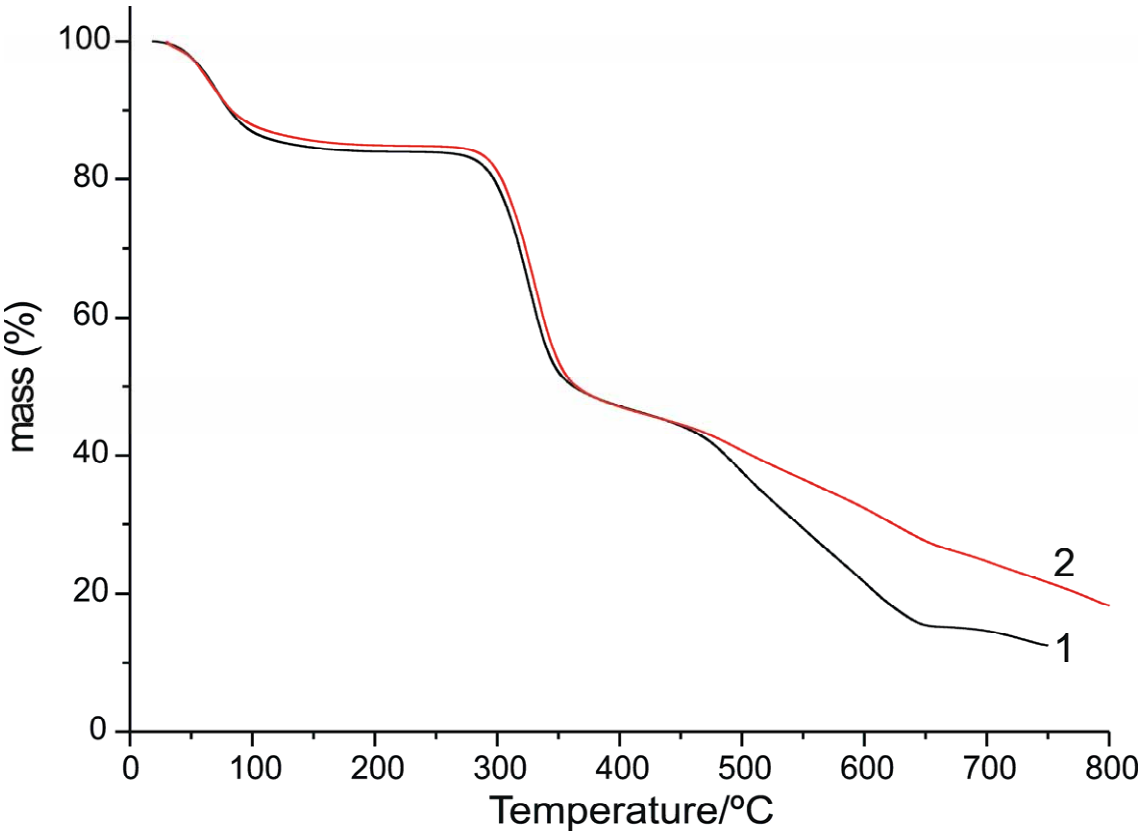

Figure S3. TGA of compounds **1**(black) and **2** (red).

2.2 – FTIR-ATR

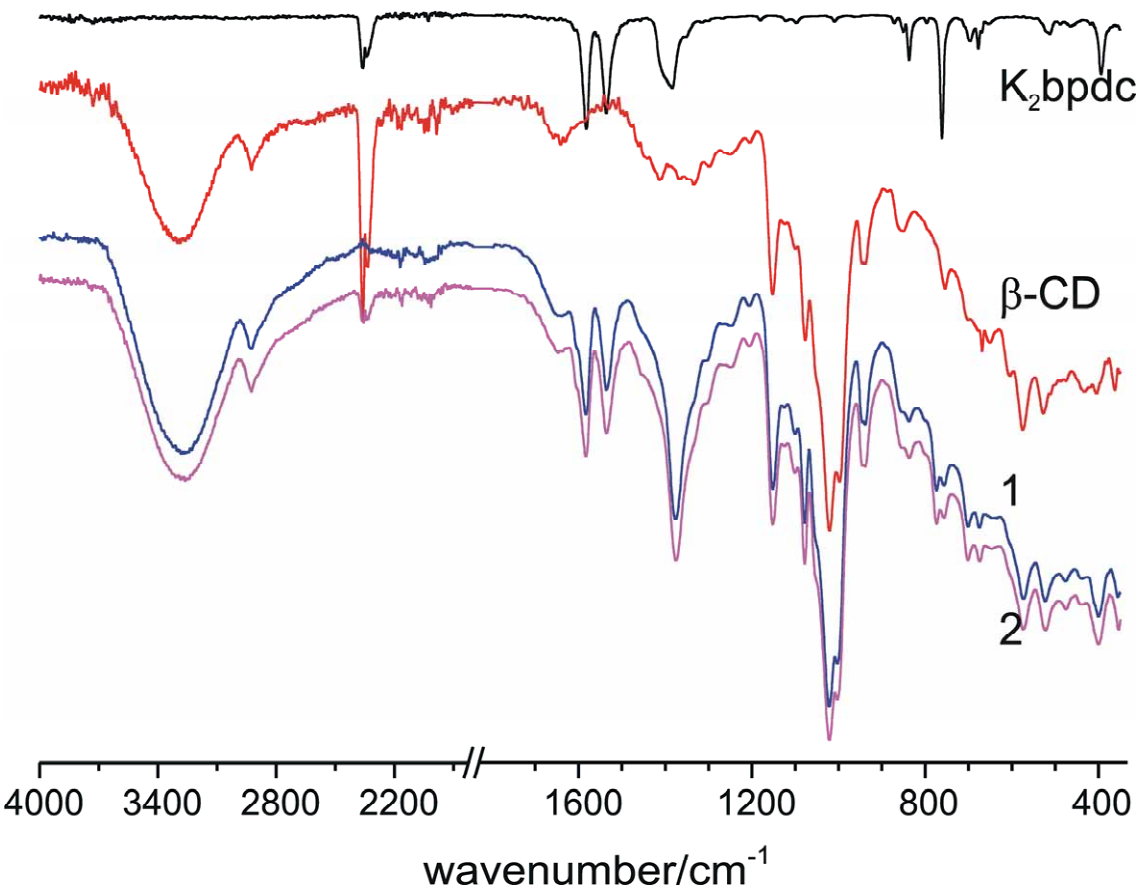

Figure S4. FT-IR ATR spectra of compounds **1** and **2**. The spectra of β-CD and K_2bpdc are also represented for comparative purposes. The two latter spectra were scaled and subject to an offset for clarity purposes.

2.3 – FT-Raman

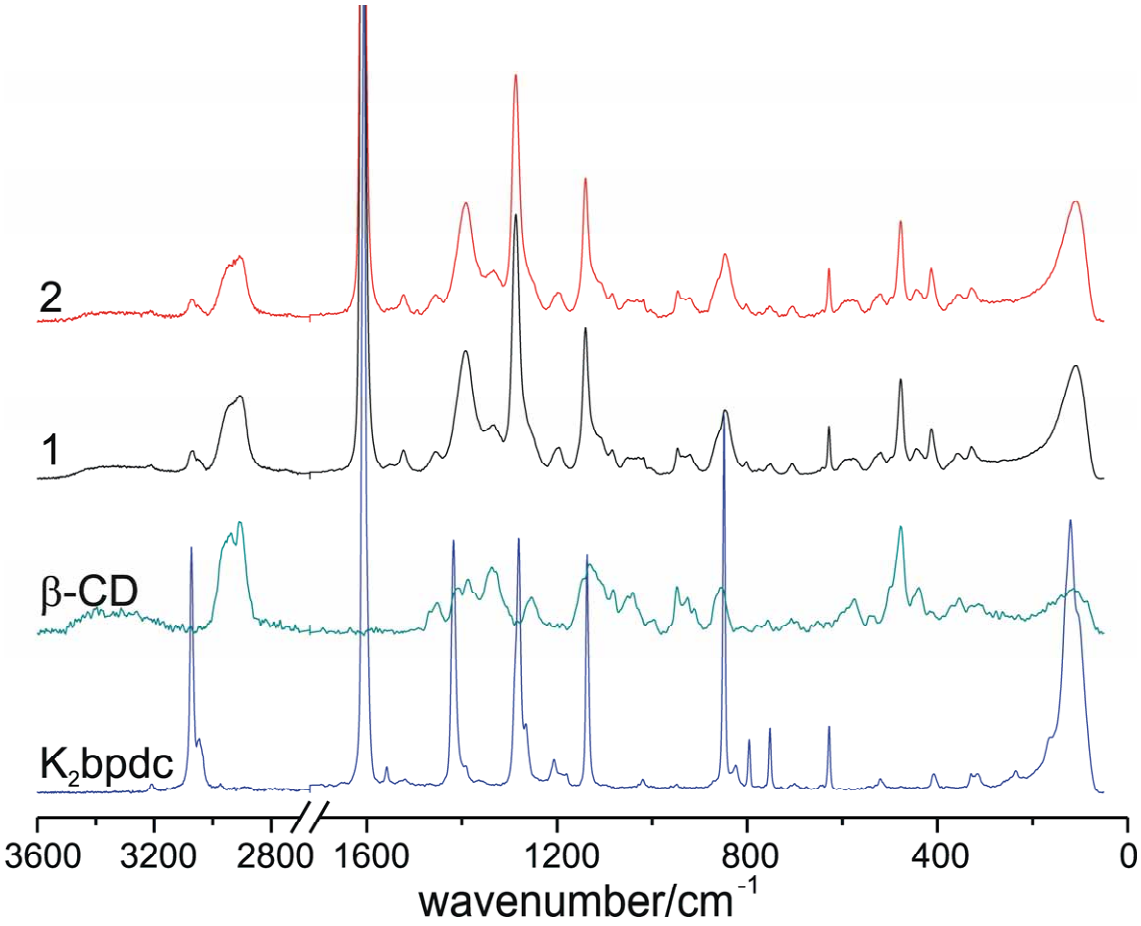

Figure S5. FT-Raman spectra of compounds **1** and **2**. The spectra of β-CD and K_2bpdc are also represented for comparison.

3 – References

1. K. K. Irikura, R. D. Johnson and R. N. Kacker, *J. Phys. Chem. A*, 2005, **109**, 8430-8437.