Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Optimised Synthesis and Further Structural Diversity of Ytterbium Benzene-1,4-Dicarboxylate MOFs

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Lattice parameters of materials

Table S1: Refined lattice parameters of Yb_6-MOF ($P\bar{1}$) from powder diffraction compared with values determined by single crystal diffraction in our previous work, Burnett *et al.*, and by Weng *et al.*

	a / Å	*b* / Å	*c* / Å	*α* / °	*β* / °	*γ* / °
Pawley analysis (this work)	11.428(6)	12.0951(21)	13.024(6)	86.876(13)	67.070(13)	72.202(7)
Single crystal (Burnett *et al.*)[1]	11.3495(2)	11.9759(2)	12.9732(2)	86.754(1)	67.067(1)	72.156(1)
Single crystal (Weng *et al.*)[2]	11.363(3)	11.989(3)	12.987(4)	86.741(4)	67.084(4)	72.150(4)

Table S2: Refined lattice parameters of UOW-3 ($P\bar{1}$) compared with values determined by single crystal diffraction in others' work

	a / Å	*b* / Å	*c* / Å	*α* / °	*β* / °	*γ* / °
UOW-3 Single crystal (this work)	7.7973(3)	9.4775(4)	10.6851(4)	68.823(4)	70.748(3)	74.995(3)
Feng *et al.*[3]	7.8413(7)	9.5545(8)	10.6561(9)	68.827(1)	71.024(1)	75.206(0)
Zehnder *et al.*[4]	7.782(2)	9.465(3)	10.681(3)	68.748(3)	70.677(3)	74.963(3)

Table S3: Refined lattice parameters of UOW-4 (*Pbca*) from powder diffraction compared with values determined by single crystal diffraction, and for the Er analogue reported by Pan *et al.*

	a / Å	*b* / Å	*c* / Å
As made UOW-4 / TWC2	9.6233(12)	26.2954(28)	37.7540(26)
Single crystal	9.59605(10)	26.1011(3)	37.7873(4)
$Er_4(BDC)_6(H_2O)_6$ (Pan *et al.*)[5]	9.661(2)	26.224(3)	37.863(3)

Table S4: Refined lattice parameters of UOW-5 ($P2_1/c$) from powder diffraction compared with values determined by single crystal diffraction.

	a / Å	*b* / Å	*c* / Å	*β* / °
Powder Diffraction	9.8467(25)	22.4394(6)	13.838(5)	108.527(10)
Single crystal	9.82977(6)	22.43648(14)	13.79565(9)	108.6081(7)

FT-IR Spectra

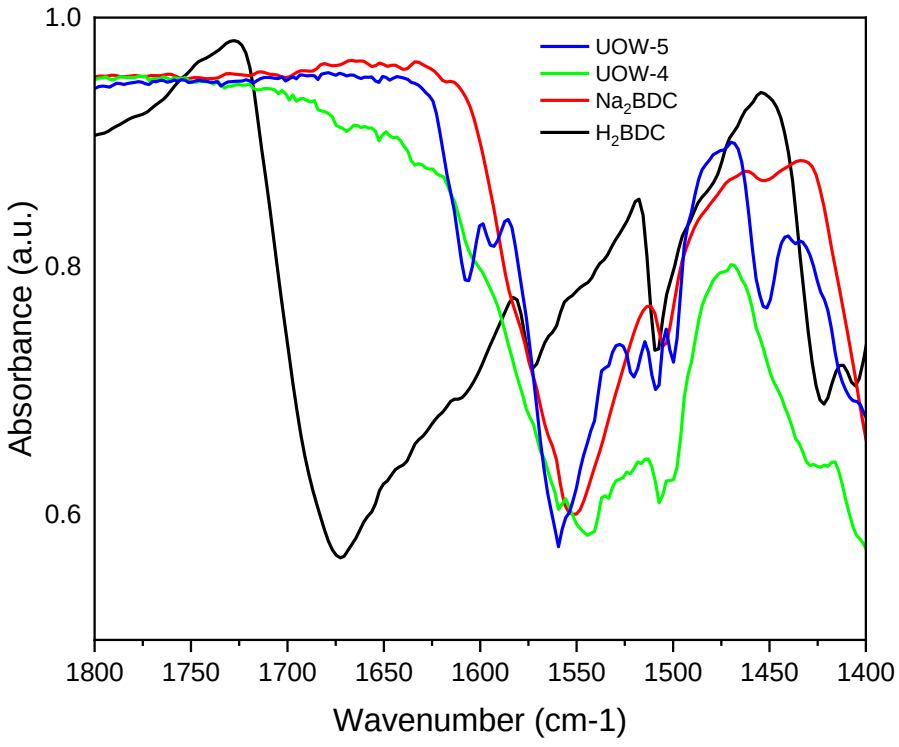

Figure S1: FT-IR spectra showing the absence of carboxylate OH features in UOW-4 compared to UOW-5.

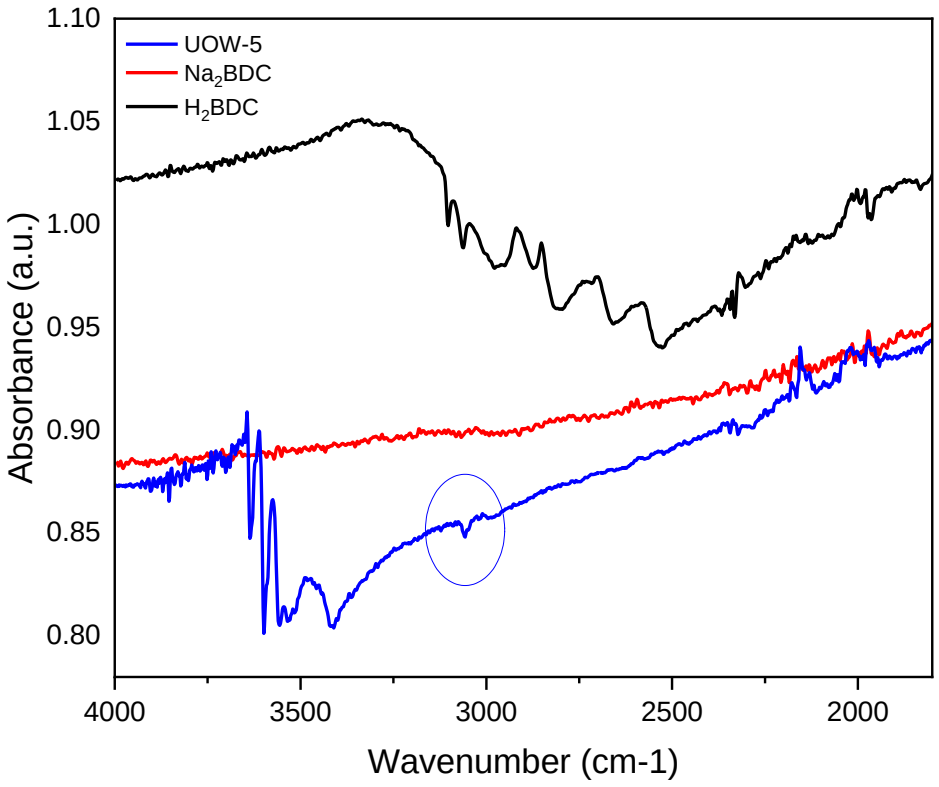

Figure S2: FT-IR spectra in the O-H stretch with carboxylate O-H indicated in UOW-5 by the circle. O-H stretches due to hydroxide ions are seen ~3700 – 3500 cm^{-1}.

REFERENCES

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