Supporting information for:

The selective intercalation of organic carboxylates and sulfonates into hydroxy double salts

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Tables

Table S1: Selective uptake of BDC isomers by Zn_5-NO_3 after reaction in water for 6 days with a 4-fold excess of each guest. Data are given as mean and standard deviation (S.D.) from three independent experiments. Percentages may not add up to 100 % owing to rounding to 1 d.p.

T / °C	% of 1,2-BDC intercalated		% of 1,4-BDC intercalated	
	Mean	S.D.	Mean	S.D.
20	4.9	0.4	95.2	0.4
40	0.7	1.2	99.3	1.2
60	1.4	1.2	98.6	1.2
80	2.0	0	98.0	0
100	2.0	0.2	98.0	0.2

Table S2: Selective uptake of BDC isomers by Zn_5-NO_3 after reaction in water for 4 days with a 4-fold excess of each guest. Data are given as mean and standard deviation (S.D.) from three independent experiments. Percentages may not add up to 100 % owing to rounding to 1 d.p.

T / °C	% of 1,2-BDC intercalated		% of 1,4-BDC intercalated	
	Mean	S.D.	Mean	S.D.
20	5.4	0.2	94.6	0.2
40	2.6	1.0	97.4	1.0
60	2.0	0	98.0	0
80	0	0	100	0
100	1.0	1.0	99.0	1.0

Table S3: Selective uptake of BDC isomers by Zn_5-NO_3 after reaction in water/acetone for 6 days with a 4-fold excess of each guest. Data are given as mean and standard deviation (S.D.) from three independent experiments. Percentages may not add up to 100 % owing to rounding to 1 d.p.

T / °C	% of 1,2-BDC intercalated		% of 1,4-BDC intercalated	
	Mean	S.D.	Mean	S.D.
20	5.4	0.3	94.6	0.3
40	4.3	0.5	95.7	0.5
60	0	0	100	0
80	1.3	1.2	98.7	1.2
100	0.7	1.2	99.3	1.2

Table S4: Selective uptake of BDC isomers by Zn_5-NO_3 after reaction in water/acetone for 4 days with a 4-fold excess of each guest. Data are given as mean and standard deviation (S.D.) from three independent experiments. Percentages may not add up to 100 % owing to rounding to 1 d.p.

T / °C	% of 1,2-BDC intercalated		% of 1,4-BDC intercalated	
	Mean	S.D.	Mean	S.D.
20	6.7	0.8	93.4	0.8
60	2.9	1.6	97.1	1.6
80	1.3	0.6	98.7	0.6
100	2.0	0	98.0	0

Table S5: Selective uptake of BDC isomers by Zn_5-NO_3 after reaction in water for 6 days with a varying excess of each guest. Data are given as mean and standard deviation (S.D.) from three independent experiments. Percentages may not add up to 100 % owing to rounding to 1 d.p.

BDC excess	T / °C	% of 1,2-BDC intercalated		% of 1,4-BDC intercalated	
		Mean	S.D.	Mean	S.D.
2-fold	20	4.2	0.6	95.8	0.6
	40	2.3	0.1	97.7	0.1
	100	1.0	1.4	99.0	1.4
1-fold	20	7.4	0.6	92.6	0.6
	40	3.0	1.3	97.0	1.3
	60	2.0	0	98.0	0
	100	0	0	100	0

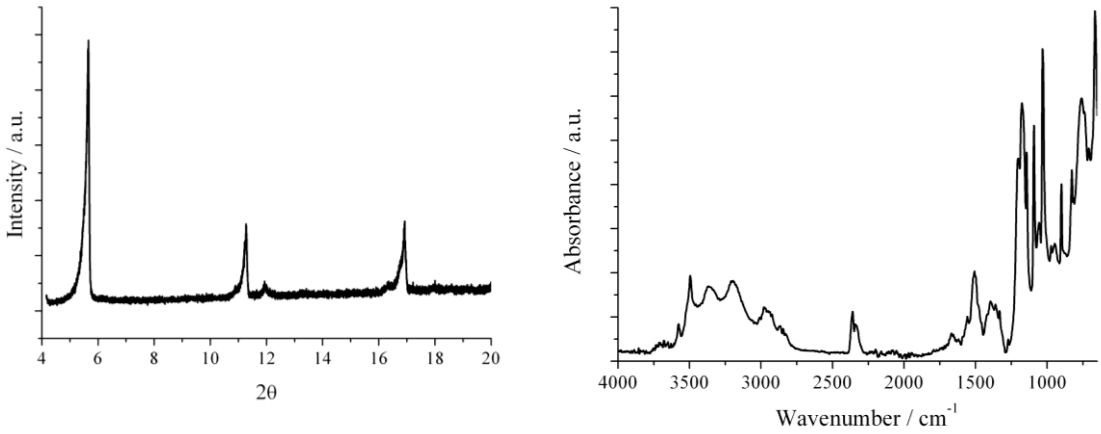
Table S6: Selective uptake of NDS isomers by Zn_5-NO_3 after reaction in water for 6 days with a 4-fold excess of each guest. Data are given as mean and standard deviation (S.D.) from three independent experiments. Percentages may not add up to 100 % owing to rounding to 1 d.p.

T / °C	% of 1,5-NDS intercalated		% of 2,6-NDS intercalated	
	Mean	S.D.	Mean	S.D.
20	0	0	100	0
40	8.2	2.1	91.8	2.1
60	0.9	1.6	99.1	1.6
80	0.2	0.3	99.8	0.3
100	3.2	1.0	96.8	1.0

Table S7: Selective uptake of NDS isomers by Zn_5-NO_3 after reaction in water for 4 days with a 4-fold excess of each guest. Data are given as mean and standard deviation (S.D.) from three independent experiments. Percentages may not add up to 100 % owing to rounding to 1 d.p.

T / °C	% of 1,5-NDS intercalated		% of 2,6-NDS intercalated	
	Mean	S.D.	Mean	S.D.
20	0	0	100	0
40	5.5	2.8	94.5	2.8
60	2.1	0.3	97.9	0.3
80	1.8	0.4	98.2	0.4
100	0.4	0.8	99.6	0.8

Figures



(a) **(b)**

Figure S1: (a) X-ray diffraction pattern and **(b)** IR spectrum for the 2,6-NDS intercalate of Zn_5-NO_3.

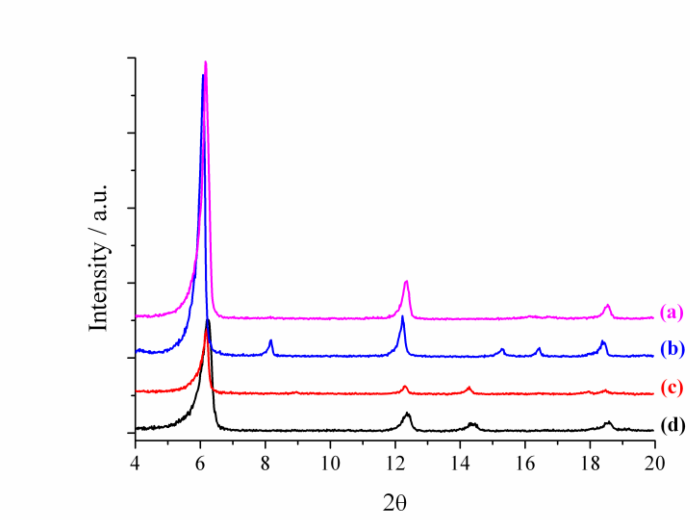


Figure S2: X-ray diffraction patterns of the 1,4-BDC intercalates of **(a)** Zn_3Ni_2-NO_3; **(b)** $Zn_{3.8}Co_{1.2}$-NO_3; **(c)** Zn_5-acetate; and, **(d)** Zn_5-Cl.

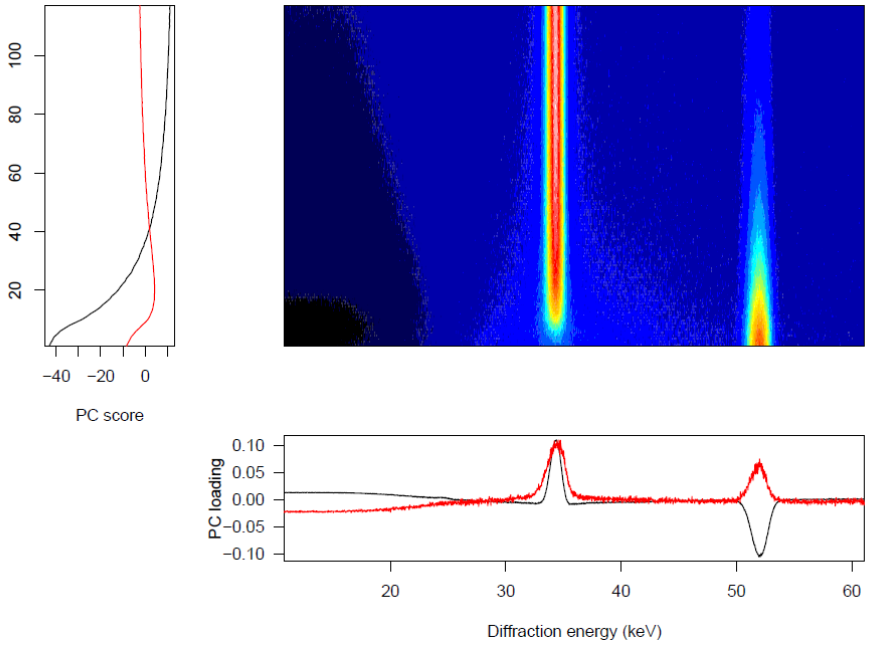


Figure S3: PCA of *in situ* EDXRD data for the intercalation of 1,4-BDC into Zn_5-NO_3 at 80 °C. Principal component (PC) 1 is shown in black, and PC2 in red.

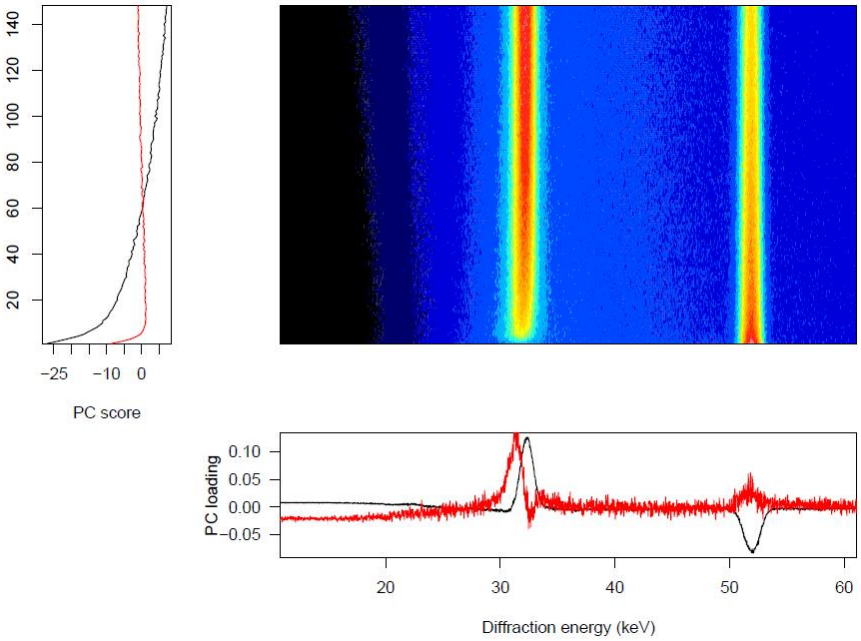


Figure S4: PCA of *in situ* EDXRD data for the intercalation of 1,2-BDC into Zn_5-NO_3 at 80 °C. Principal component (PC) 1 is shown in black, and PC2 in red.

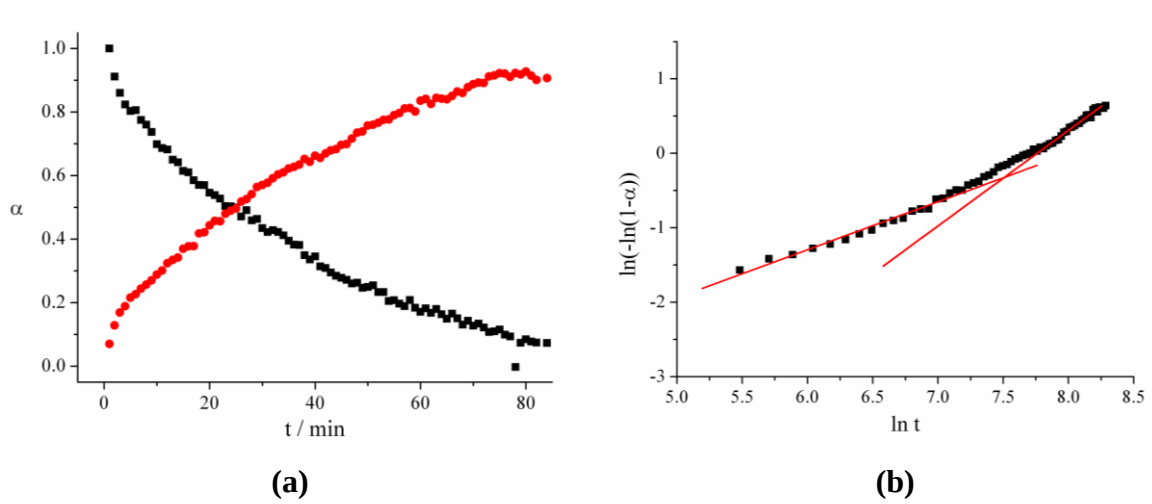


Figure S5: EDXRD data for the intercalation of 1,2-BDC into Zn_5-NO_3 at 90 °C. **(a)** Extent of reaction *vs*. time plots for the *200* reflections of Zn_5-NO_3 (■) and Zn_5-1,2-BDC (●). **(b)** Sharp-Hancock plot showing the discontinuity in mechanism.

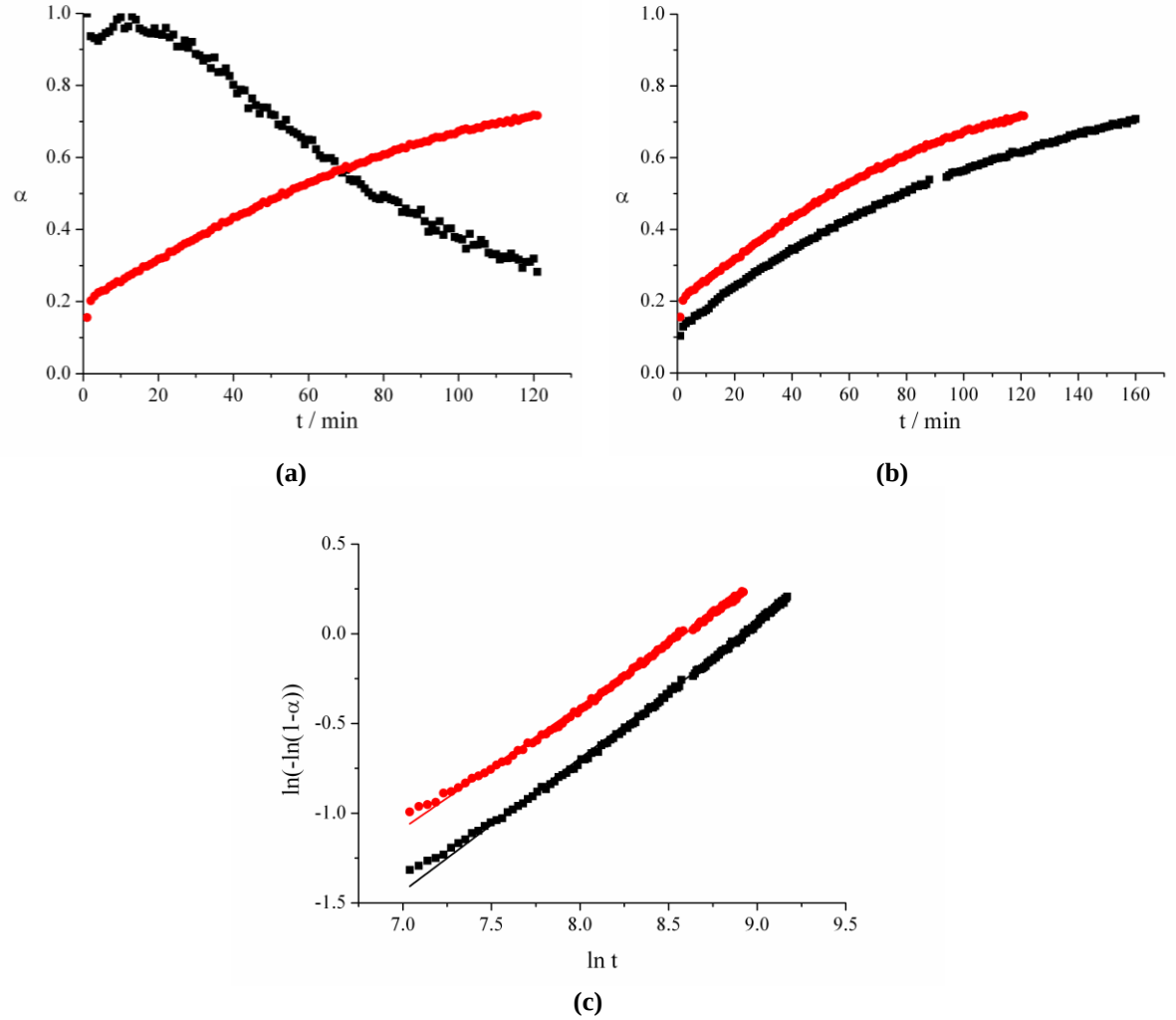


Figure S6: EDXRD data for the intercalation of 1,4-BDC into Zn_5-Cl. **(a)** Extent of reaction *vs*. time plots for the *200* reflections of Zn_5-Cl (■) and Zn_5-1,4-BDC (●) at 90 °C. **(b)** Extent of reaction *vs.* time plots showing the growth of the Zn_5-1,4-BDC *200* reflection at 80 (■) and 90 °C (●). **(c)** Sharp-Hancock plots at at 80 (■) and 90 °C (●).

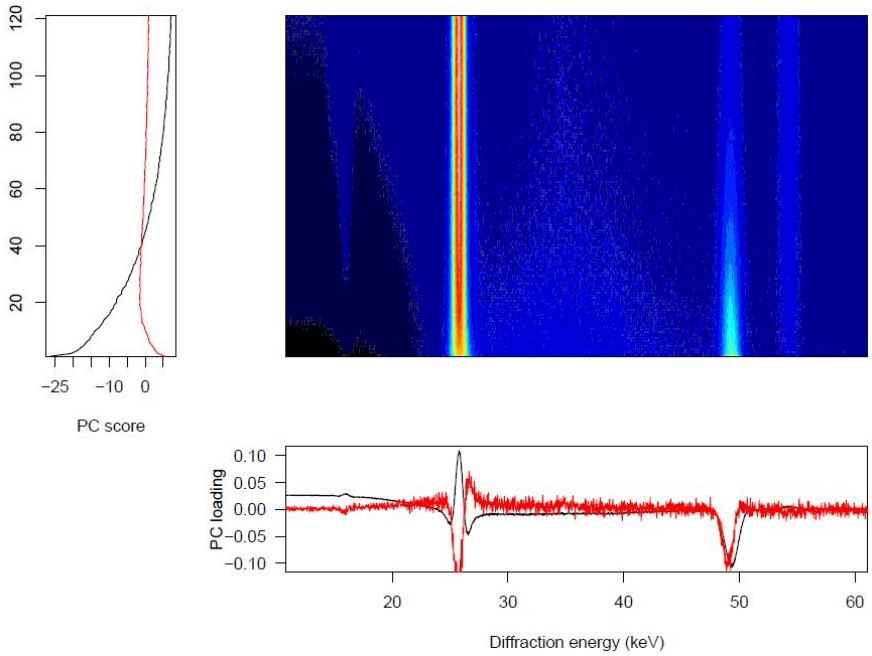


Figure S7: PCA of *in situ* EDXRD data for the intercalation of 1,4-BDC into Zn_5-Cl at 90 °C. Principal component (PC) 1 is shown in black, and PC2 in red.

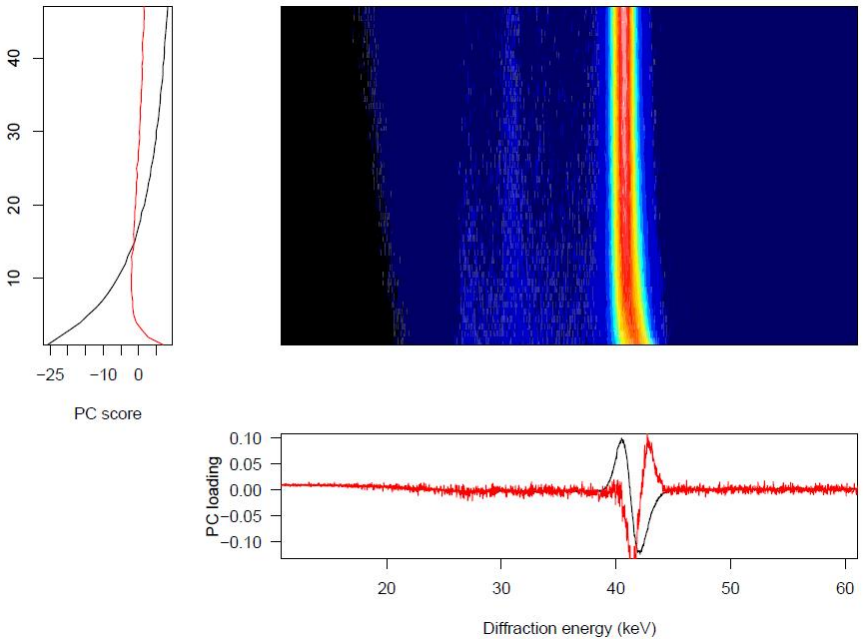


Figure S8: PCA of *in situ* EDXRD data for the intercalation of 1,2-BDC into Zn_5-acetate at 90 °C. Principal component (PC) 1 is shown in black, and PC2 in red

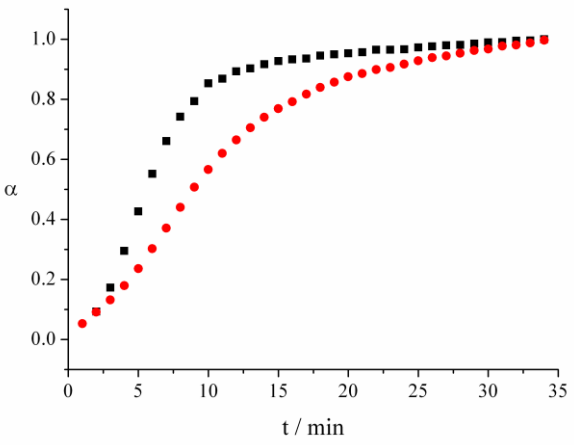


Figure S9: EDXRD data for the intercalation of 1,2-BDC and 1,4-BDC into $Zn_{3.8}Co_{1.2}$-NO_3 showing the growth in the *200* reflections of $Zn_{3.8}Co_{1.2}$-1,2-BDC (■) and $Zn_{3.8}Co_{1.2}$-1,4-BDC (●) at 80 °C.

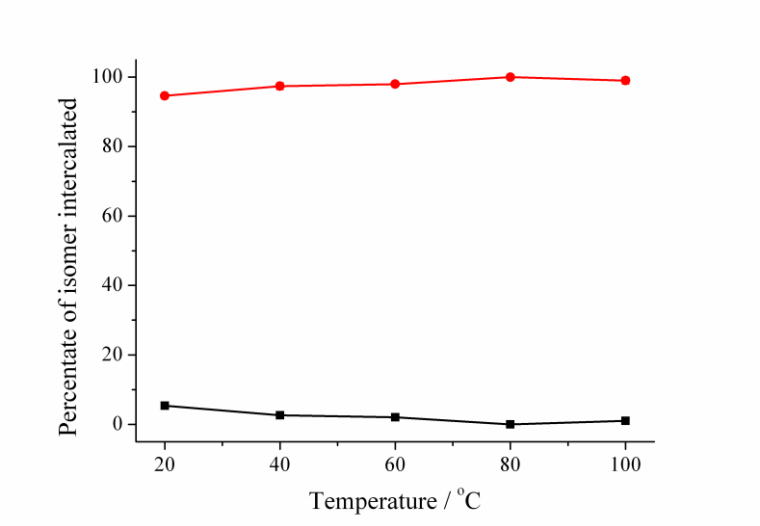


Figure S10: The results of the competitive intercalation of 1,2- (■) and 1,4-BDC (●) into Zn_5-NO_3 for 4 days in water, with a 4-fold excess of each guest used. Experiments were performed in triplicate and mean ± S.D. are plotted (error bars are so small as to be contained within the points on the graph here).

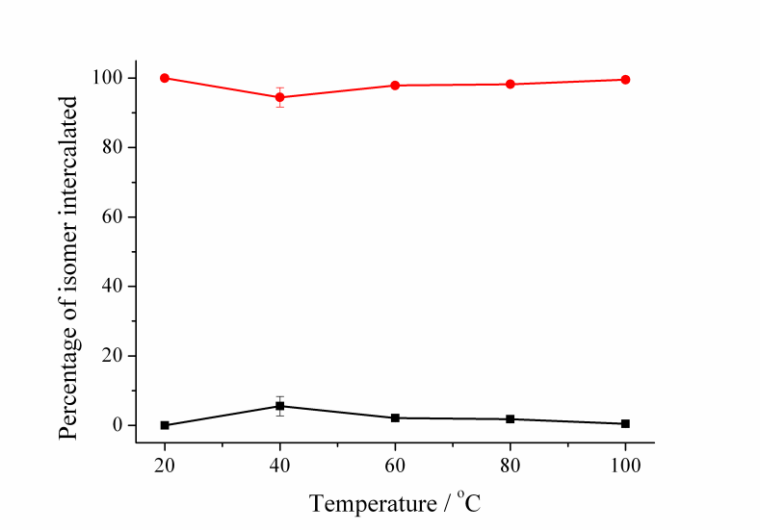


Figure S11: The results of the competitive intercalation of 1,5- (■) and 2,6-NDS (●) into Zn_5-NO_3 for 4 days in water, with a 4-fold excess of each guest used. Experiments were performed in triplicate and mean ± S.D. are plotted (error bars are so small as to be mostly contained within the points on the graph).

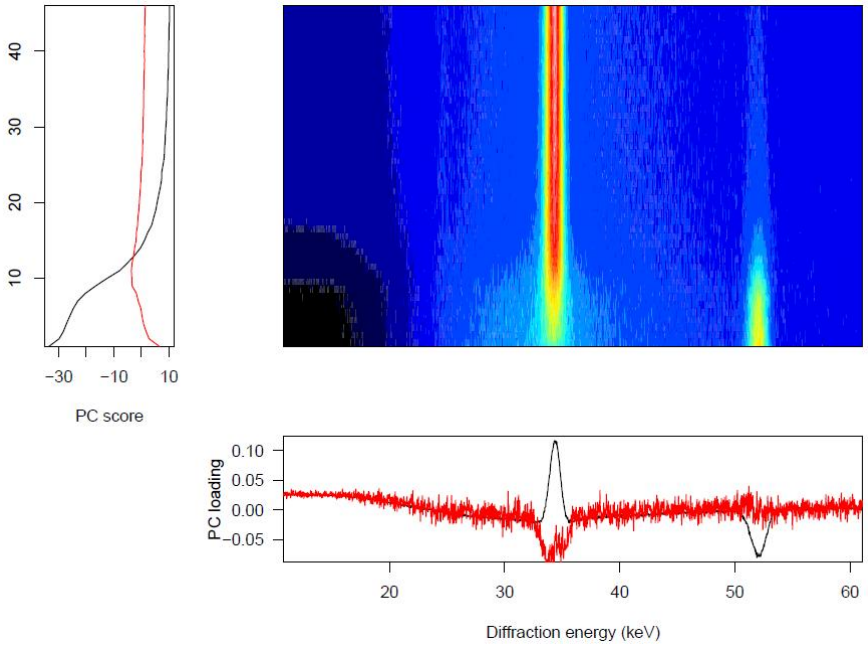


Figure S12: PCA of *in situ* EDXRD data for the intercalation of a mixture of 1,2- and 1,4-BDC into Zn_5-NO_3 at 90 °C. Principal component (PC) 1 is shown in black, and PC2 in red.