Supporting Information for:

Nickel(II) Metal-Organic Frameworks with N,N'-di(4-pyridyl)-1,4,5,8-naphthalenetetracarboxydiimide Ligands: Influence of Secondary Building Unit Geometry on Dimensionality and Framework Dimensions.

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Table S1. Bond lengths and angles for **1**.

Bond	Oxygen ligand	Bond Length (Å)	Angle	Oxygen ligand	Angle (°)	Angle	Oxygen ligand	Angle (°)
Ni1–N1[b]	N/A	2.058(7)	O3–Ni1–O3[1]	DMF	178.8(3)	O4A–Ni1–O3	Nitrate/DMF	82.4(4)
Ni1–N4[2]	N/A	2.078(7)	O3–Ni1–N4[2]	DMF	90.59(14)	O4A[1]–Ni1–N1	Nitrate	89.2(4)
Ni1–O3	DMF	2.075(6)	O3[1]–Ni1–N4[2]	DMF	90.59(14)	O4A–Ni1–N1	Nitrate	89.2(4)
Ni1–O3[1]	DMF	2.075(6)	O3–Ni1–N1	DMF	89.41(14)	O4A[1]–Ni1–N4[2]	Nitrate	90.8(4)
Ni1–O4A	Nitrate	2.046(9)	O3[1]–Ni1–N1	DMF	89.41(14)	O4A–Ni1–N4[2]	Nitrate	90.8(4)
Ni1–O4A[1]	Nitrate	2.046(9)	O4A–Ni1–O3[1]	Nitrate/DMF	97.6(4)	O4A[1]–Ni1–O4A	Nitrate	178.4(8)
			O4A[1]–Ni1–O3[1]	Nitrate/DMF	82.4(4)	N1–Ni1–N4[2]	N/A	180
			O4A[1]–Ni1–O3	Nitrate/DMF	97.6(4)			

[a]For the disordered ligands (DMF and nitrate molecules) the highest occupancy molecule was used. [b]N designates the DPNDI ligand. [1] and [2] designate different ligands.

Table S2. Bond lengths for **2** and **3**.

	2	**3**
Bond	**Bond Length (Å)**	**Bond Length (Å)**
Ni–N[i] (DPNID pyridine)	2.084 (2)	2.081 (2)
Ni–N[ii] (DPNID pyridine)	2.087 (2)	2.091 (2)
Ni–O[i] (carboxylic acid)	1.9836 (19)	1.993 (2)
Ni–O[ii] (carboxylic acid)	2.0087 (18)	1.9945 (18)
Ni–O[i] (nitrate)	2.1299 (19)	2.153 (2)
Ni–O[ii] (nitrate)	2.159 (2)	2.1738 (19)

*[i] and [ii] designate atoms from different ligands

Table S3. Bond Angles for **2** and **3**.

	2	**3**
Bonds	**Angle (°)**	**Angle (°)**
N[i]–Ni–O[i] (carboxylic acid)	86.90 (8)	88.47 (9)
N[i]–Ni–O[ii] (carboxylic acid)	89.19 (9)	96.57 (8)
N[i]–Ni–O[i] (nitrate)	88.72 (8)	87.32 (8)
N[i]–Ni–O[ii] (nitrate)	89.30 (8)	90.79 (9)
N[ii]–Ni–O[i] (carboxylic acid)	89.99 (9)	88.62 (8)
N[ii]–Ni–O[i] (carboxylic acid)	95.70 (8)	89.00 (9)
N[ii]–Ni–O[i] (nitrate)	88.33 (8)	88.37 (8)
N[ii]–Ni–O[ii] (nitrate)	91.03 (9)	89.57 (9)
N[i]–Ni–N[ii]	177.40 (9)	174.81 (9)

*N designates a nitrogen atom on the pyridine group of the DPNDI molecule. [i] and [ii] designate atoms from different ligands.

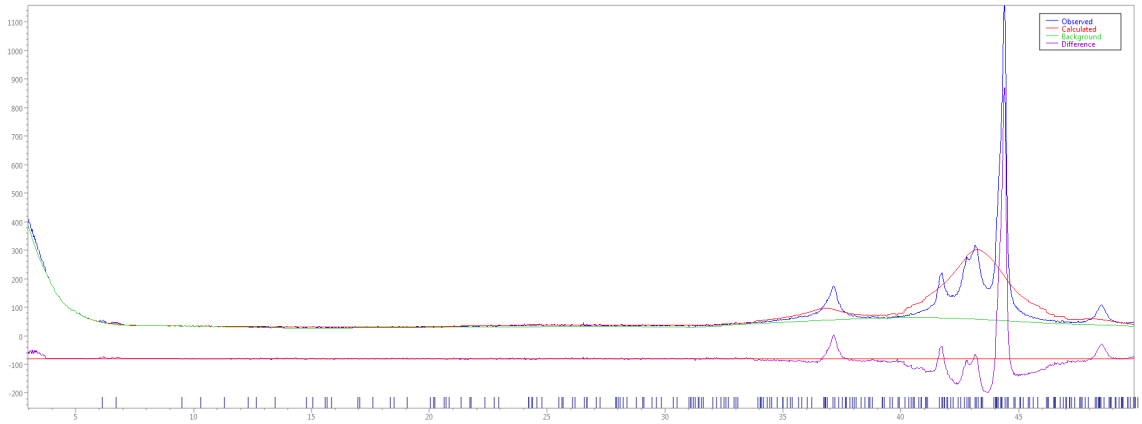

Fig. S1. PXRD pattern for **1**. Observed experimental diffractogram – blue trace. Pattern indicates significant loss of crystallinity upon drying.

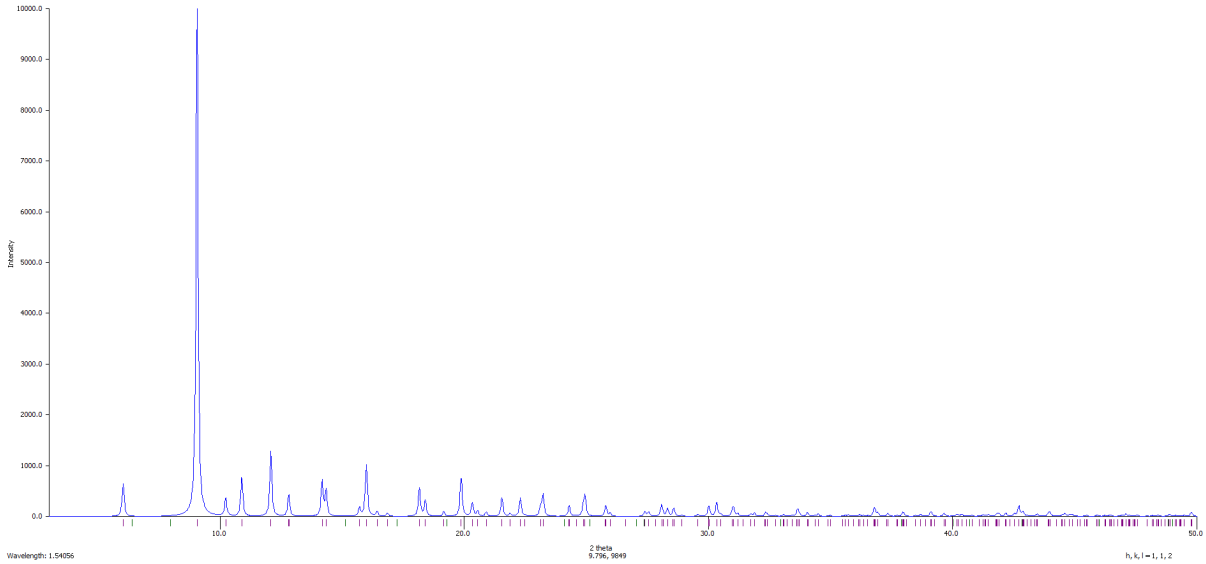

Fig. S2. Calculated PXRD pattern for **1**. Calculated using Mercury.[S1]

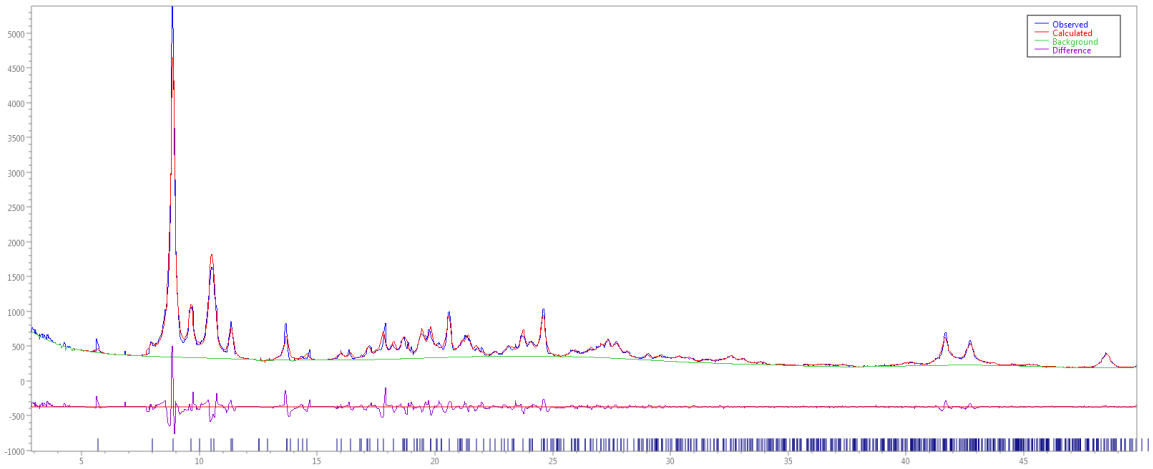

Fig. S3. PXRD pattern for **2**. Observed experimental diffractogram – blue trace; calculated pattern in red.

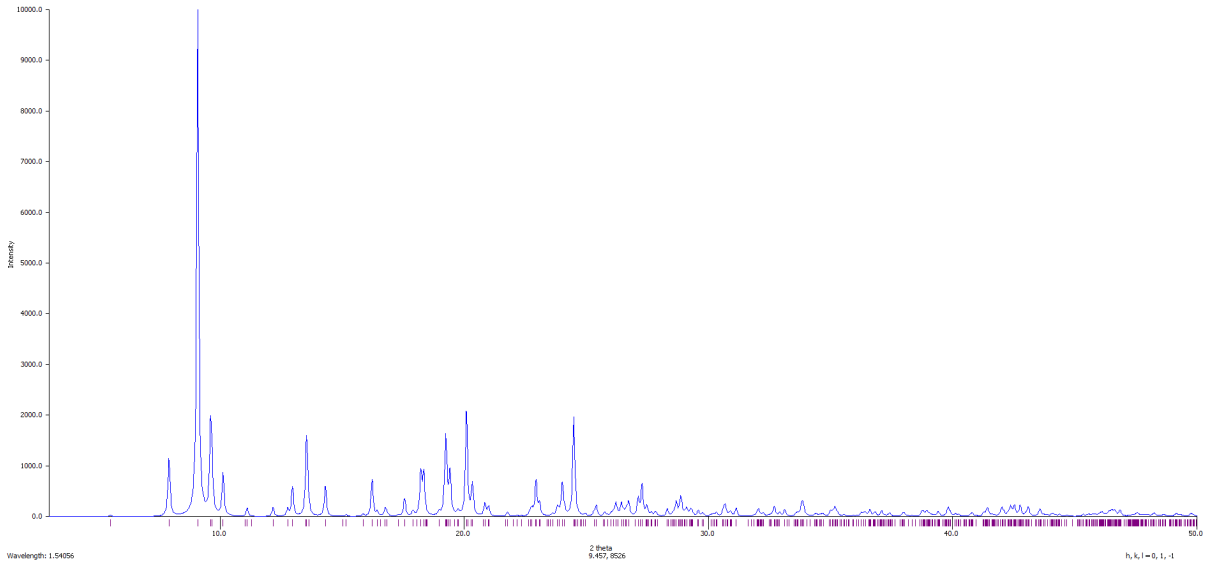

Fig. S4. Calculated PXRD pattern for **2**. Calculated using Mercury.[S1]

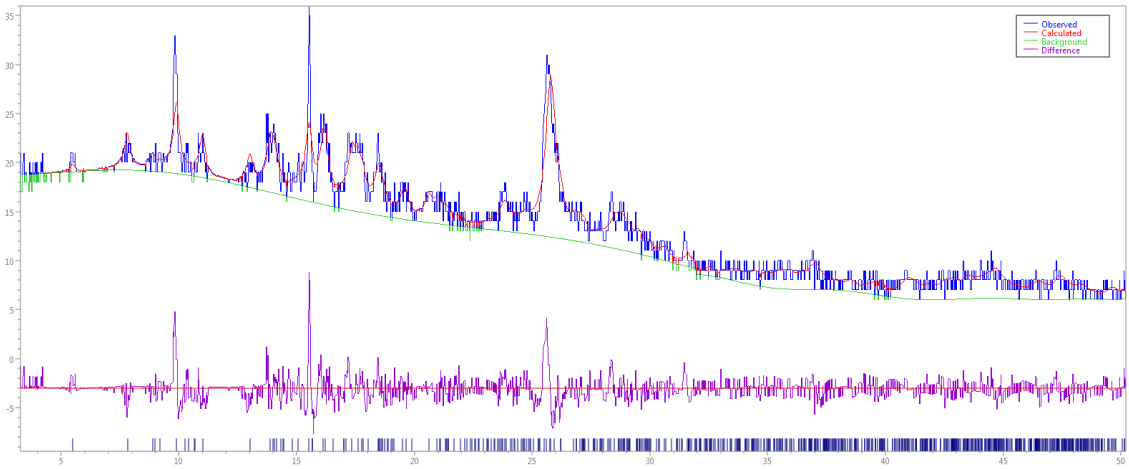

Fig. S5. PXRD pattern for **3**. Observed experimental diffractogram – blue trace; calculated pattern in red. Pattern indicates low crystallinity of sample upon drying.

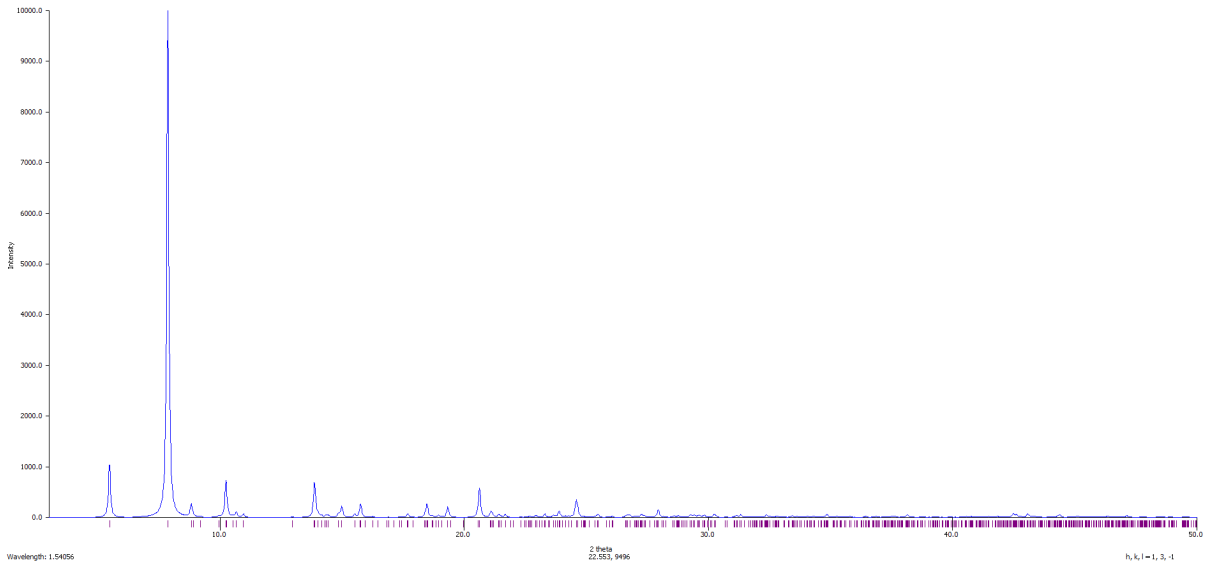

Fig. S6. Calculated PXRD pattern for **3**. Calculated using Mercury.[S1]

References

S1. C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. van de Streek and P. A. Wood, *J. Appl. Cryst.*, 2008, **41**, 466-470.