

Electronic Supplementary Information

Construction of highly energetic metal-organic frameworks with a nitrobenzene derivative

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General procedures: All reagents and solvents were of the analytical reagent grade and used without further purification. C, H and N analyses were made on an Elementar Vario-EL CHNS elemental analyzer. Fourier transform infrared spectra were obtained on a NICOLET iS 50 spectrometer with sample prepared as KBr discs in the range of 4000–400 cm^{-1} . Powder X-ray diffraction (PXRD) patterns of samples **1-3** were collected on a Bruker D8 ADVANCE X-Ray Diffractometer (Cu-K α , $\lambda = 1.54056 \text{ \AA}$) in the in the 2θ range of 5-50° with a scan speed of 0.2 sec/deg. Thermogravimetical analyses (TGA) were performed in N₂ atmosphere on a simultaneous STA 449-F5 thermal analyzer from 25 °C up to 800 °C with a heating rate of 5-20 °C/min.

Table S1 Selected Bond Lengths (Å) and Bond Angles (°) in **1-3**

1					
Cd1-O2	2.326(3)	Cd1-O9	2.185(3)	Cd1-O10	2.239(3)
O9-Cd1-O2	96.81(10)	O10-Cd1-O2	160.28(10)	O11-Cd1-O2	82.45(10)
O2-Cd1-O2	69.89(10)	O9-Cd1-O3	87.87(10)	O10-Cd1-O3	91.95(10)
O11-Cd1-O3	175.19(10)	O2-Cd1-O3	68.46(9)	O2-Cd1-O3	97.23(10)
2					
Cud1-O11A	1.958(4)	Cu1-O6	2.385(4)	Cu2-O12B	1.829(10)
Cu2-O12A	1.932(11)	Cu2-O9	1.943(7)	Cu2-O9	1.961(7)
2.003(11)	2.003(11)	Cu2-O12B	2.048(10)		
O2-Cu1-O2	180.0	O2-Cu1-O11A	88.58(16)	O2-Cu1-O11A	91.42(16)
O2-Cu1-O11A	88.58(16)	O11A-Cu1-O11A	180.0	O3-Cd1-O1	113.09(13)
O2-Cu1-O6	101.07(15)	O2-Cu1-O6	78.93(15)	O11A-Cu1-O6	94.60(15)
O11A-Cu1-O6	85.40(15)	O2-Cu1-O6	101.07(15)	O6-Cu1-O6	180.0
O12B-Cu2-O12A	19.1(3)	O12B-Cu2-O9	92.2(4)	O12A-Cu2-O9	94.7(4)
O9-Cu2-O9	165.53(14)	O12B-Cu2-O12A	174.0(4)	O12A-Cu2-O12A	165.78(16)
O12A-Cu2-O9	84.2(4)	O12A-Cu2-O9	92.0(4)	O12B-Cu2-O12B	166.9(2)
O12A-Cu2-O12B	148.0(3)	O9-Cu2-O12B	86.8(4)	O9-Cu2-O12B	85.3(4)
3					
Nd1-O2B	2.325(5)	O2A-Nd1-O9A#1	133.72(16)	O10B#2-Nd1-O11C	69.5(4)
Nd1-O2A	2.390(5)	O11A-Nd1-O9A#1	81.94(18)	O2B-Nd1-O3A	136.76(17)
Nd1-O11A	2.397(5)	O11B-Nd1-O9A#1	73.84(17)	O2A-Nd1-O3A	63.94(15)
Nd1-O11B	2.429(5)	O2B-Nd1-O10B#2	143.38(19)	O11A-Nd1-O3A	66.37(16)
Nd1-O9A#1	2.441(5)	O2A-Nd1-O10B#2	86.74(16)	O11B-Nd1-O3A	134.15(16)
Nd1-O10B#2	2.444(4)	O11A-Nd1-O10B#2	135.31(16)	O9A#1-Nd1-O3A	69.78(15)
Nd1-O11X	2.47(3)	O11B-Nd1-O10B#2	76.02(17)	O10B#2-Nd1-O3A	69.45(16)
Nd1-O11C	2.521(14)	O9A#1-Nd1-O10B#2	76.98(16)	O11X-Nd1-O3A	124.0(8)
Nd1-O3A	2.685(5)	O2B-Nd1-O11X	67.3(8)	O11C-Nd1-O3A	120.0(4)
Nd1-O3B	2.781(5)	O2A-Nd1-O11X	71.2(8)	O2B-Nd1-O3B	62.89(16)
O9A-Nd1#3	2.441(5)	O11A-Nd1-O11X	135.9(8)	O2A-Nd1-O3B	139.26(16)
O10B-Nd1#4	2.444(4)	O11B-Nd1-O11X	73.4(8)	O11A-Nd1-O3B	68.45(17)
O2B-Nd1-O2A	86.55(17)	O9A#1-Nd1-O11X	141.8(8)	O11B-Nd1-O3B	66.51(17)
O2B-Nd1-O11A	78.48(18)	O10B#2-Nd1-O11X	76.5(8)	O9A#1-Nd1-O3B	67.73(15)
O2A-Nd1-O11A	80.08(18)	O2B-Nd1-O11C	74.2(5)	O10B#2-Nd1-O3B	133.89(16)
O2B-Nd1-O11B	88.46(18)	O2A-Nd1-O11C	72.0(4)	O11X-Nd1-O3B	115.0(8)

O2A-Nd1-O11B	143.32(17)	O11A-Nd1-O11C	141.7(5)	O11C-Nd1-O3B	119.2(4)
O11A-Nd1-O11B	134.17(18)	O11B-Nd1-O11C	71.7(5)	O3A-Nd1-O3B	120.72(15)
O2B-Nd1-O9A#1	130.56(16)	O9A#1-Nd1-O11C	136.4(5)		

Symmetry codes: #1 $x+1/2, y-1/2, z$ #2 $x-1, -y+1, z-1/2$ #3 $x-1/2, y+1/2, z$ #4 $x+1, -y+1, z+1/2$