Supplementary Materials: Flexible Yttrium Coordination Geometry Inhibits "Bare-Metal" Guest Interactions in the Metal-Organic Framework Y(btc)

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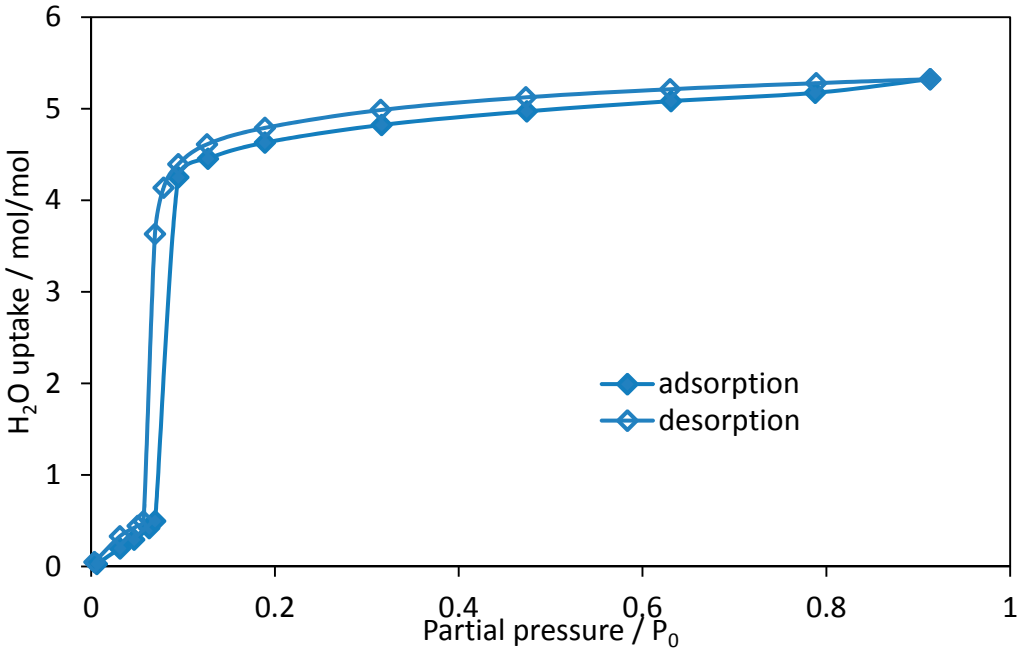

Figure S1. Water vapour adsorption isotherm for the Y(btc) framework at 298 K. Filled points indicate the adsorption scan, open points the desorption scan. Note that at the step the kinetics were extremely slow, and several points were omitted as equilibrium values could not be reliably extrapolated.

Table S1. Rietveld refinement results for the Y(btc) framework dosed with 1 CO_2:Y. See Table 1 for refined parameters of the guest atoms.

Atom	Site Description	Fractional Coordinates			Fractional Occupancy [1]	U_{iso} (10^{-2} Å^2)
		x (*a*)	*y* (*b*)	*z* (*c*)		
Y1	Framework	0.3787(10)	0.3787(10)	0.125	1	5.0(4)
O1		0.2294(18)	0.428(2)	1.0091(14)	1	11.8(7)
O2		0.4211(12)	0.4016(12)	0.9109(7)	1	3.4(4)
O3		0.8128(9)	0.5902(10)	0.6916(7)	1	2.3(3)
C1		0.2779(7)	0.5	0.75	1	3.3(4)
H1A		0.404(2)	0.5	0.75	1	4.0(8)
C2		0.2130(5)	0.4554(10)	0.8325(3)	1	2.5(3)
C3		0.0806(6)	0.4593(9)	0.8339(3)	1	2.3(3)
H3A		0.0486(15)	0.4383(15)	0.8958(9)	1	1.3(4)
C4		0.0171(6)	0.5	0.75	1	1.0(3)
C5		0.2948(8)	0.4283(10)	0.9207(6)	1	3.9(3)
C6		0.8761(15)	0.5	0.75	1	3.4(5)

[1] Fixed to 1 where not specified.

Table S2. Rietveld refinement results for the Y(btc) framework dosed with 2 CO_2:Y.

Atom	Site Description	Fractional Coordinates			Fractional Occupancy [1]	U_{iso} (10^{-2} Å^2)
		x (*a*)	*y* (*b*)	*z* (*c*)		
Y1	Framework	0.376(2)	0.376(2)	0.125	1	5.5(10)
O1		0.217(3)	0.433(4)	1.0185(15)	1	17.9(19)
O2		0.410(3)	0.407(3)	0.9199(15)	1	7.6(12)
O3		0.8119(18)	0.591(2)	0.6833(12)	1	3.7(7)
C1		0.2793(13)	0.5	0.75	1	2.9(8)
H1A		0.413(5)	0.5	0.75	1	2.4(15)
C2		0.2151(11)	0.458(2)	0.8329(6)	1	3.7(6)
C3		0.0824(13)	0.452(2)	0.8316(8)	1	4.5(8)
H3A		0.050(3)	0.438(3)	0.8963(17)	1	0.3(7)
C4		0.0181(13)	0.5	0.75	1	0.6(6)
C5		0.2944(17)	0.432(3)	0.9207(12)	1	5.5(8)
C6		0.877(3)	0.5	0.75	1	5.8(11)
C1a	A_{CO_2}	0.804(4)	0.859(7)	0.372(5)	0.476(21)	12(3)
O1a		0.821(7)	0.895(7)	0.447(4)	0.476(21)	12(3)
O1b		0.842(6)	0.829(9)	0.302(5)	0.476(21)	12(3)
C2a	B_{CO_2}	0.671(14)	0.0	0.25	0.37(4)	17(7)
O2a		0.700(14)	−0.045(11)	0.174(5)	0.37(4)	17(7)
C3a	C_{CO_2}	1.0	0.916(15)	0.5	0.27(3)	9(4)
O3a		0.899(8)	0.966(12)	0.536(6)	0.27(3)	9(4)

[1] Fixed to 1 where not specified.

Table S3. Rietveld refinement results for the Y(btc) framework dosed with 2 CD_4:Y.

Atom	Site Description	Fractional Coordinates			Fractional Occupancy [1]	U_{iso} (10^{-2} Å^2)
		x (*a*)	*y* (*b*)	*z* (*c*)		
Y1	Framework	0.3837(10)	0.3837(10)	0.125	1	2.9(4)
O1		0.2462(18)	0.4350(17)	1.0059(17)	1	9.7(7)
O2		0.4285(11)	0.4000(13)	0.9094(8)	1	2.6(4)
O3		0.8109(11)	0.5860(13)	0.6905(8)	1	3.7(4)
C1		0.2802(7)	0.5	0.75	1	1.9(4)
H1A		0.402(3)	0.5	0.75	1	7.4(12)
C2		0.2157(6)	0.4513(8)	0.8301(3)	1	0.9(3)
C3		0.0846(6)	0.4618(9)	0.8337(3)	1	1.4(3)
H3A		0.0525(15)	0.4489(16)	0.8952(11)	1	0.5(4)
C4		0.0205(7)	0.5	0.75	1	1.7(4)
C5		0.2986(7)	0.4203(9)	0.9168(7)	1	0.8(3)
C6		0.8798(14)	0.5	0.75	1	1.4(5)
C1a	A_{CD_4}	0.1617(16)	0.941(3)	0.2269(19)	0.371(7)	22.0(16)
D1a		0.234(4)	0.920(6)	0.272(4)	0.371(7)	22.0(16)
D1b		0.198(5)	0.965(5)	0.167(3)	0.371(7)	22.0(16)
D1c		0.120(6)	0.858(5)	0.207(5)	0.371(7)	22.0(16)
D1d		0.103(5)	1.003(7)	0.2493(18)	0.371(7)	22.0(16)
C2a	B_{CD_4}	0.826(2)	0.7326(17)	0.0666(13)	0.505(12)	39(3)
D2a		0.899(4)	0.670(4)	0.058(7)	0.505(12)	39(3)
D2b		0.854(3)	0.819(6)	0.036(8)	0.505(12)	39(3)
D2c		0.818(10)	0.747(11)	0.1331(16)	0.505(12)	39(3)
D2d		0.745(5)	0.705(4)	0.042(8)	0.505(12)	39(3)

[1] Fixed to 1 where not specified.

Table S4. Rietveld refinement results for the Y(btc) framework dosed with 2 O_2:Y.

Atom	Site Description	Fractional Coordinates			Fractional Occupancy [1]	U_{iso} (10^{-2} Å^2)
		x (*a*)	*y* (*b*)	*z* (*c*)		
Y1	Framework	0.3720(6)	0.3720(6)	0.125	1	1.6(3)
O1		0.2357(10)	0.4234(12)	1.0079(8)	1	6.6(4)
O2		0.4227(9)	0.4033(10)	0.9034(6)	1	4.1(3)
O3		0.8105(7)	0.5888(7)	0.6919(6)	1	1.9(3)
C1		0.2804(5)	0.5	0.75	1	1.5(3)
H1A		0.389(2)	0.5	0.75	1	5.3(7)
C2		0.2162(4)	0.4585(8)	0.8331(3)	1	3.6(2)
C3		0.0840(5)	0.4594(7)	0.8338(3)	1	3.4(2)
H3A		0.0477(11)	0.4363(10)	0.9053(7)	1	0.3(3)
C4		0.0205(5)	0.5	0.75	1	4.0(4)
C5		0.3000(5)	0.4192(6)	0.9218(4)	1	0.38(19)
C6		0.8729(10)	0.5	0.75	1	1.1(3)
O1a	A_{O_2}	0.131(4)	0.712(4)	0.055(3)	0.64(3)	28(3)
O1b		0.141(5)	0.810(4)	0.106(3)	0.64(3)	28(3)
O2a	B_{O_2}	0.818(9)	0.777(9)	0.084(5)	0.34(3)	32(7)
O3a	C_{O_2}	0.891(5)	0.870(5)	0.5868(11)	0.45(2)	26(3)

[1] Fixed to 1 where not specified.