Supporting Information

^{113}Cd NMR as a Probe of Structural Dynamics in a Flexible Porous Framework Showing Selective O_2/N_2 and CO_2/N_2 Adsorption

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Table S1: Bond length (Å) and angle (°) table for compound **1**.

Cd1-O1	2.319(5)	Cd1-O2	2.273(5)
Cd1-O3	2.502(6)	Cd1-O4	2.416(6)
Cd1-N1	2.283(5)	Cd1-O4_b	2.672(6)
O1-Cd1 -O2	95.78(10)	O1-Cd1-O3	78.62(8)
O1-Cd1-O4	169.91(9)	O1-Cd1-N1	90.61(10)
O1-Cd1-O4_b	114.12(9)	O1-Cd1-O5_b	83.18(10)
O2-Cd1-O3	54.55(10)	O2-Cd1-O4	85.12(10)
O2-Cd1-N1	147.70(12)	O2-Cd1-O4_b	120.54(10)
O2-Cd1-O5_b	85.25(11)	O3-Cd1-O4	93.89(9)
O3-Cd1-N1	96.24(10)	O3-Cd1-O4_b	167.24(8)
O3-Cd1-O5_b	133.09(9)	O4-Cd1-N1	83.44(10)
O4-Cd1-O4_b	73.55(9)	O4-Cd1-O5_b	106.92(10)
O4_b-Cd1-N1	84.72(10)	O5_b-Cd1-N1	127.00(10)
O4_b-Cd1-O5_b	51.90(9)		

Cd1-O1	2.346(10)	Cd1-O2	2.404(10)
Cd1-O3	2.351(10)	Cd1-O4	2.377(10)

Cd1-N1	2.297(10)	Cd1-O4_c	2.754(11)
Cd1-O5_c	2.234(10)	O1-Cd1-O2	97.5(3)
O1-Cd1-O3	86.1(3)	O1-Cd1-O4	170.5(2)
O1-Cd1-N1	86.9(3)	O1-Cd1-O4_c	109.8(2)
O1-Cd1-O5_c	82.8(3)	O2-Cd1-O3	54.8(3)
O2-Cd1-O4	87.9(3)	O2-Cd1-N1	152.7(3)
O2-Cd1-O4_c	119.5(3)	O2-Cd1-O5_c	82.6(3)
O3-Cd1-O4	90.6(2)	O3-Cd1-N1	99.0(3)
O3-Cd1-O4_c	164.1(2)	O3-Cd1-O5_c	134.0(2)
O4-Cd1-N1	84.8(3)	O4-Cd1-O4_c	73.9(2)
O4-Cd1-O5_c	105.8(3)	O4_c-Cd1-N1	83.4(3)
O5_c-Cd1-N1	124.7(3)	O4_c-Cd1-O5_c	50.7(2)

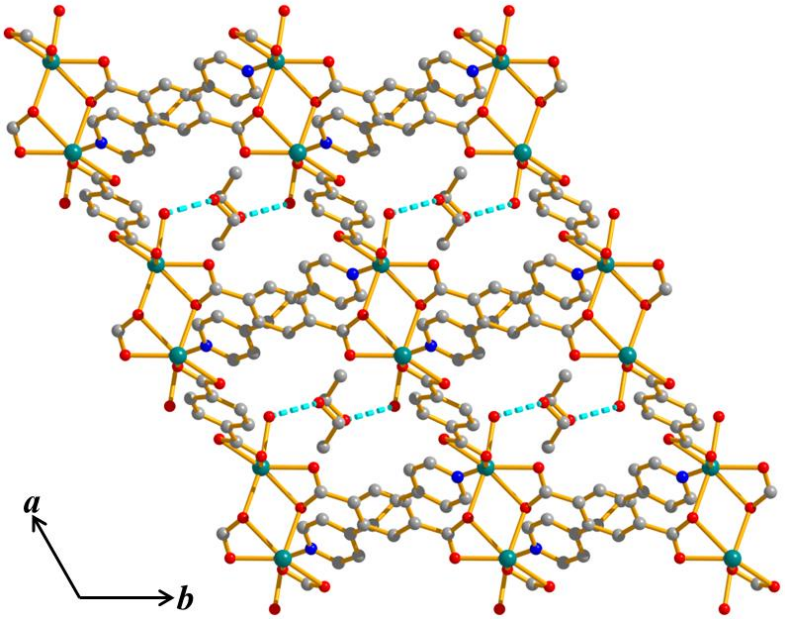

Figure S1: View of hydrogen bonding interactions in compound **1** between metal coordinated O1 and hydrogens of O6 from ethanol molecules. (Dotted cyan bonds represent hydrogen bonds).

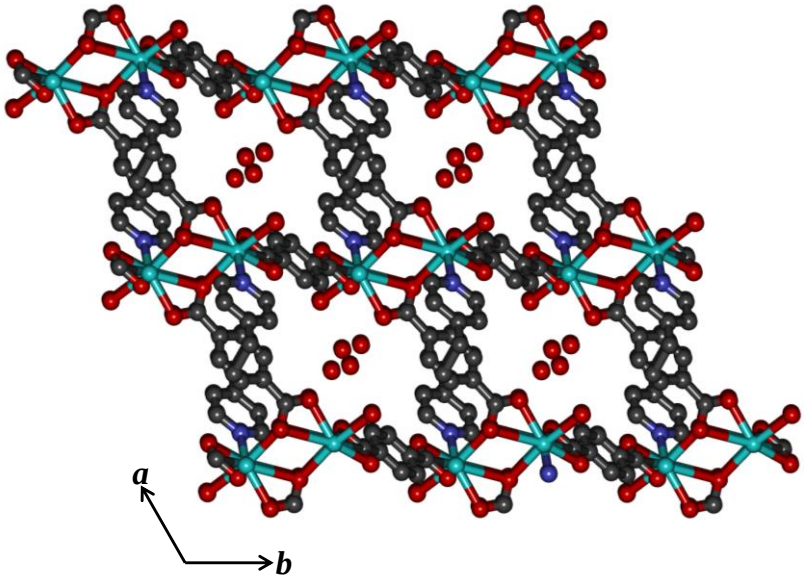

Figure S2: View of guest water molecules in compound **2** along *c*-direction.

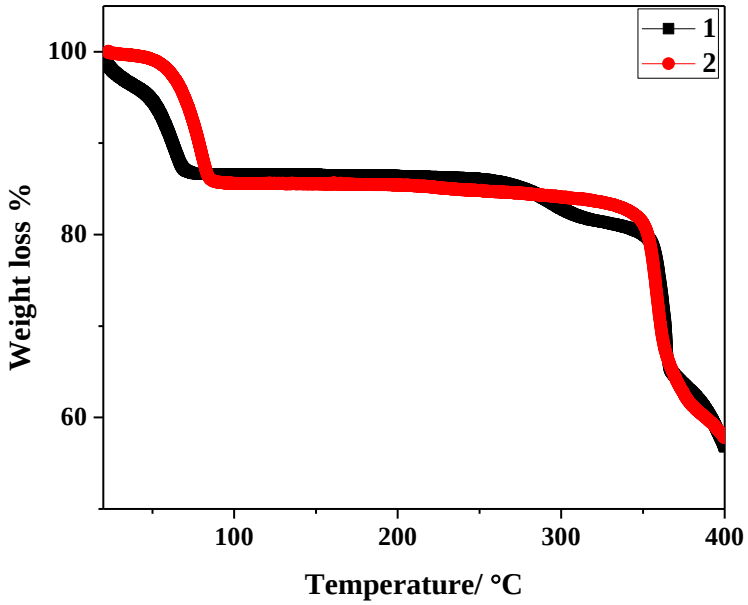

Figure S3: TG analysis of compound **1** and **2** under N_2 atmosphere with heating rate of 2 °C/min in the temperature range of 30-400 °C.

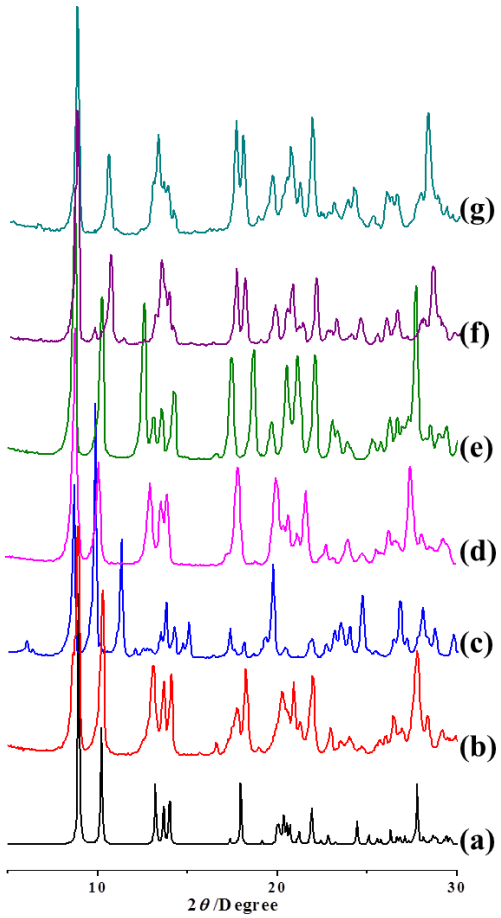

Figure S4: PXRD patterns of compound **1** (a) simulated, (b) as-synthesized, (c) desolvated, (d) ethanol, (e) water, (f) acetonitrile, (g) THF.

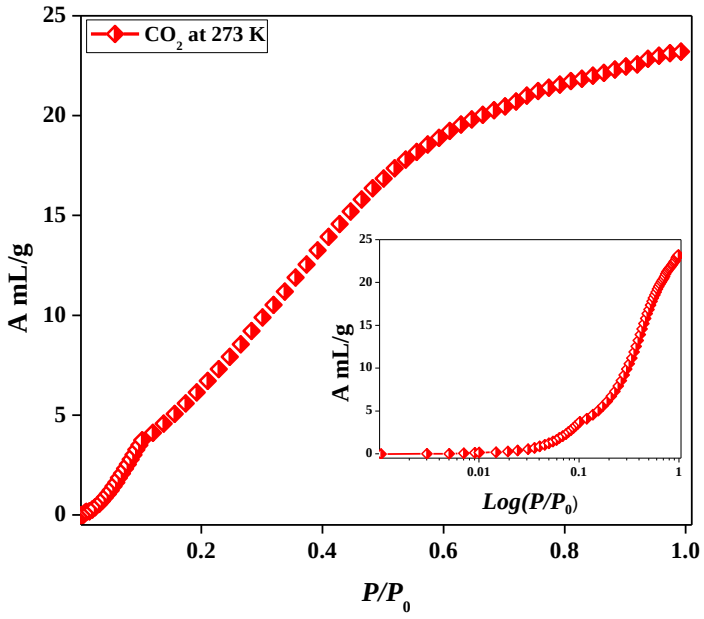

Figure S5: CO_2 adsorption isotherm of compound **1a** at 273 K; Inset shows the logarithmic pressure scale plot.