Supporting information

Selective CO_2 adsorption in four Zinc (II) based metal organic frameworks constructed by using rigid N,N′-donor linker and various dicarboxylate ligands

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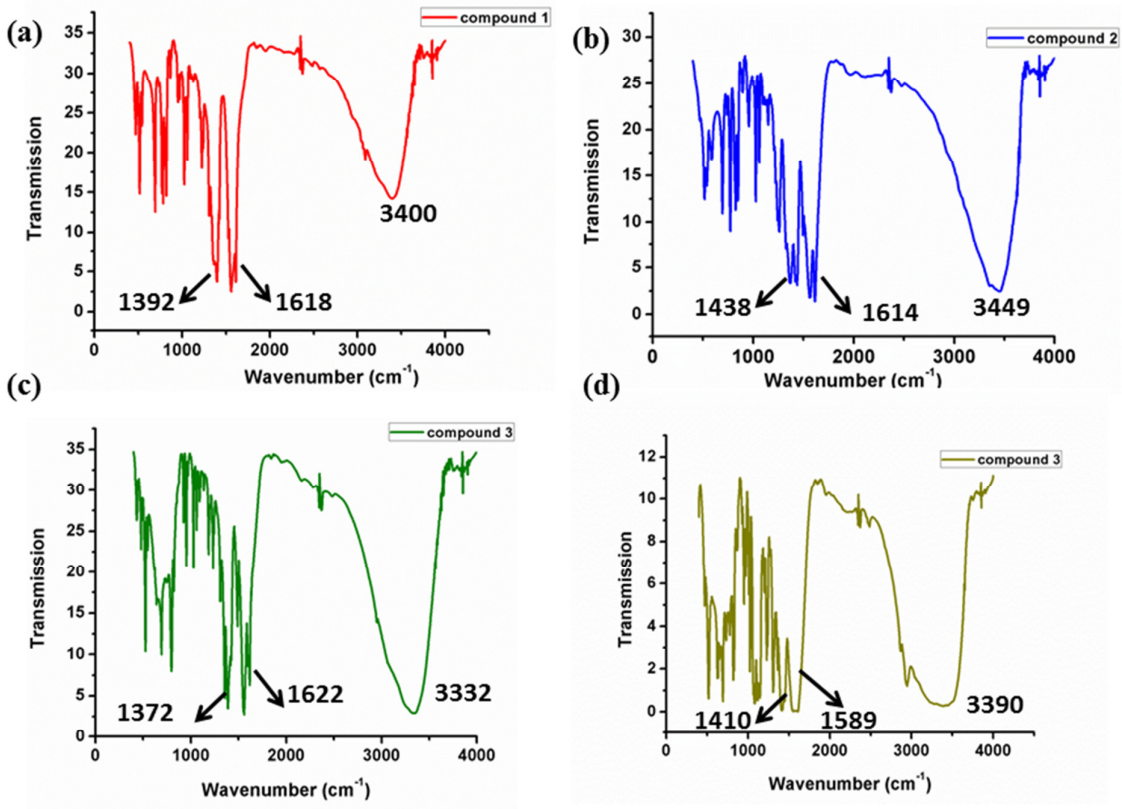

Figure S1. FT-IR spectra of compounds **1**-**4**.

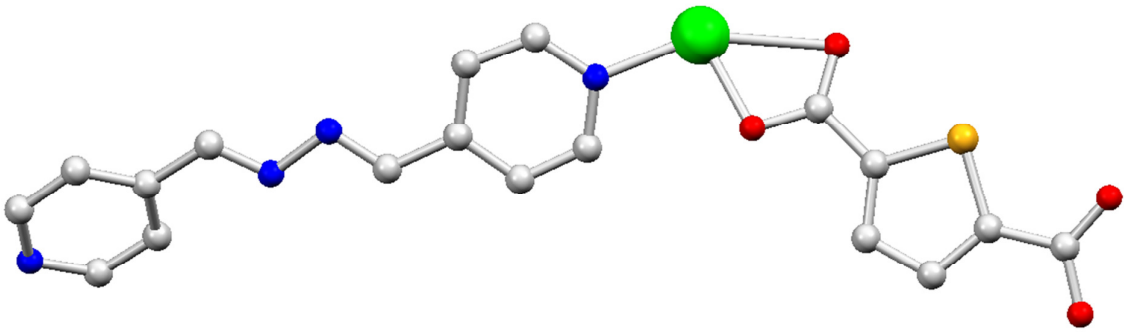

Figure S2. Asymetric unit of **1**. Color code: carbon (light gray), nitrogen (blue), oxygen (red) sulfur (yellow) and zinc (green). (Hydrogens and water molecules are omitted for clarity).

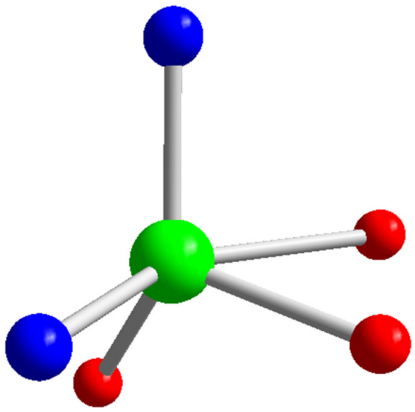

Figure S3. A distorted trigonal bipyramidal geometry of Zn(II) atom found in **1**. Color code; same as in Figure S2.

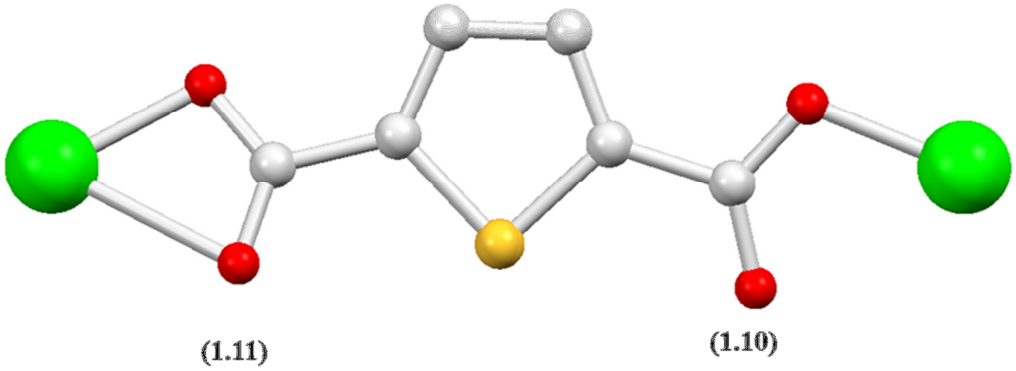

Figure S4. Bridging Modes of tdc ligand found in compound **1** (Harris Notation). Color code; same as in Figure S2.

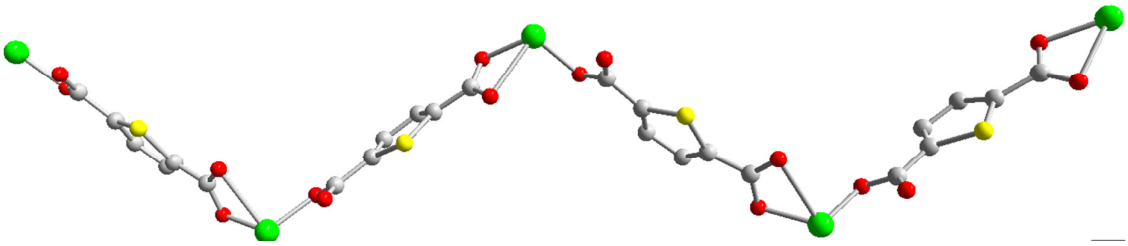

Figure S5. Illustration of 1D zig-zag chain along the *c*-axis. Color code; same as in Figure S2.

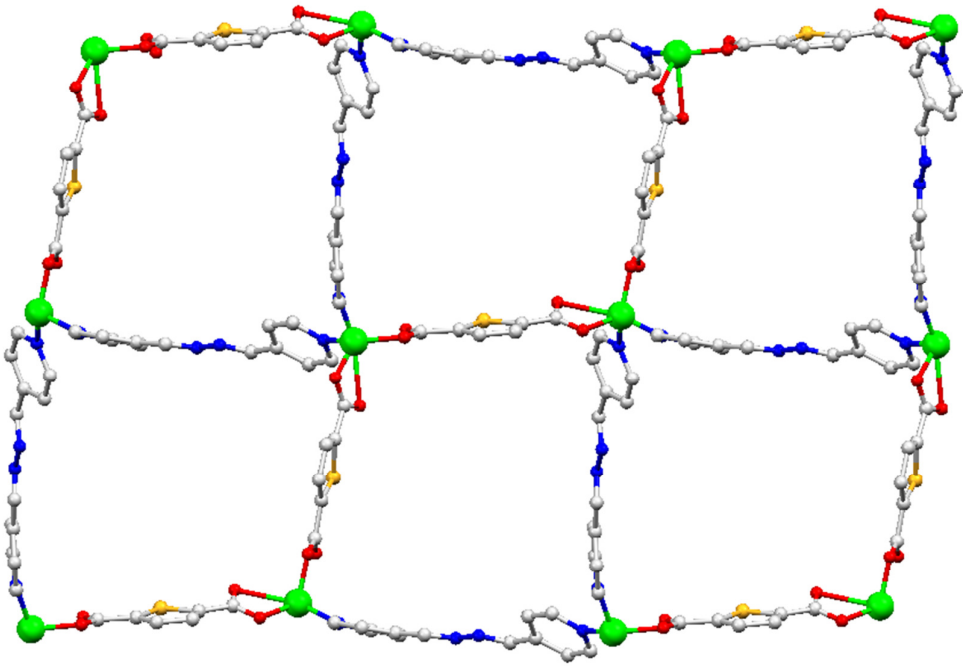

Figure S6. Illustration of 2d sheet like network along the *b*-axis. Color code; same as in Figure

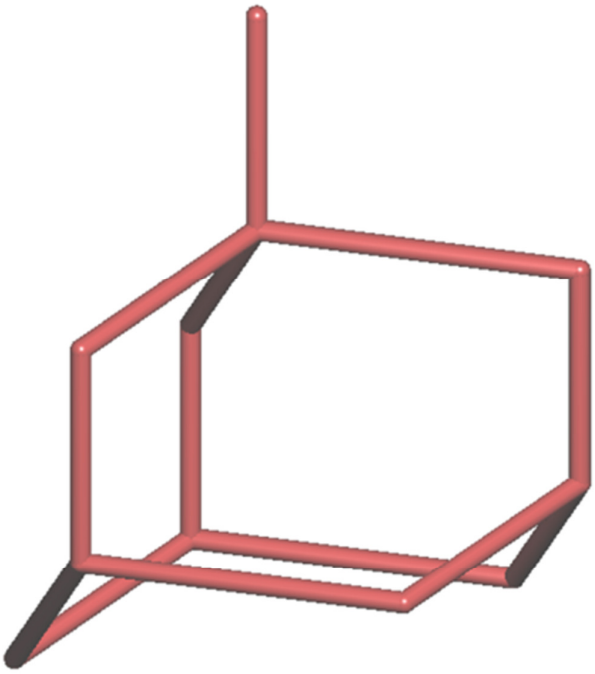

Figure S7. Simplified view of 4-connected single diamondoid (dia) topology

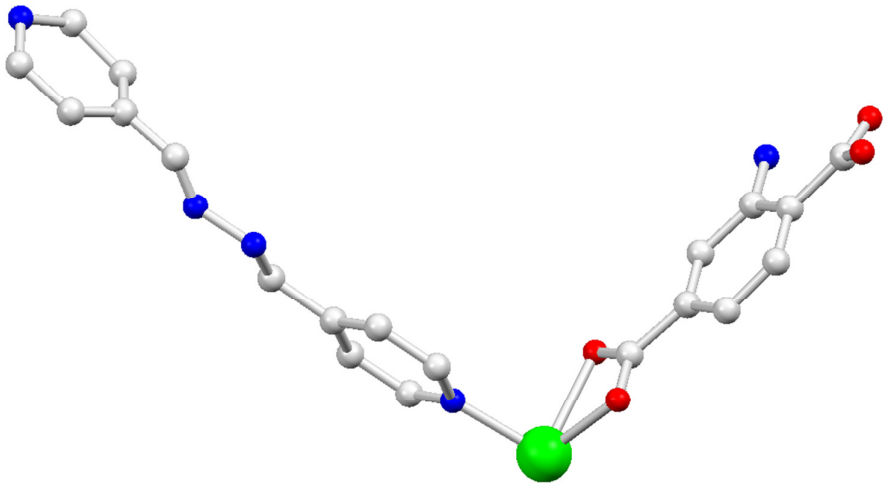

Figure. S8. Asymetric unit of **2**. Color code; same as in Figure S2. (Hydrogens and ethanol molecules are omitted for clarity).

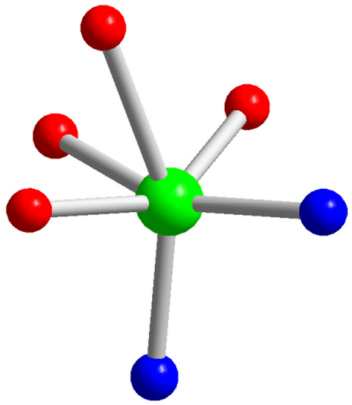

Figure S9. Highly distorted octahedral geometry of Zn(II) atom in compound **2**. Color code; same as in Figure S2.

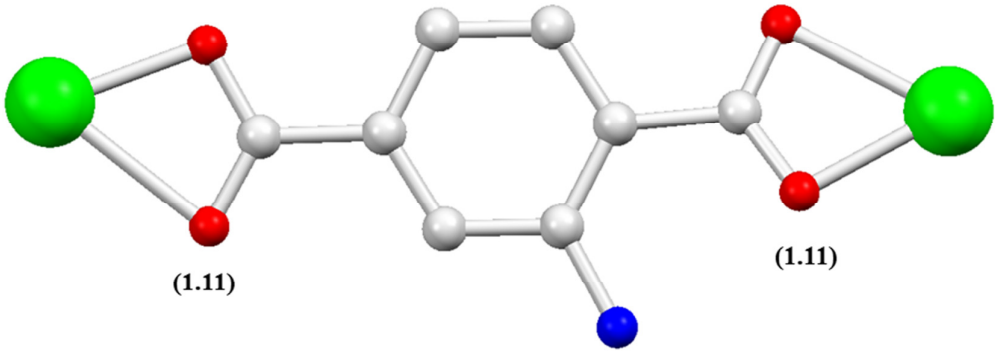

Figure S10. Bridging Mode of 2-NH_2BDC found in compound **2** (Harris Notation). Color code; same as in Figure S2.

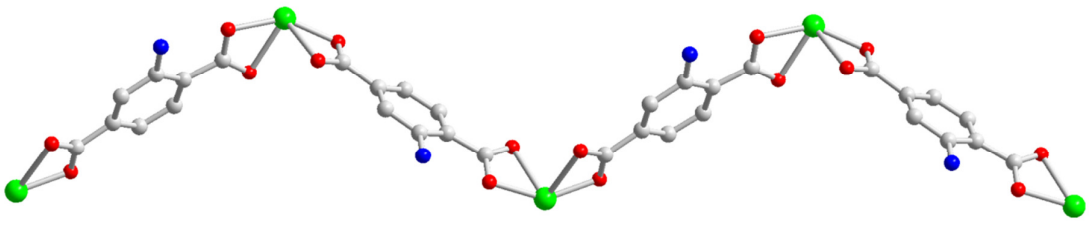

Figure S11. Illustration of 1D zig-zag chain along the *c*-axis. Color code; same as in Figure S2.

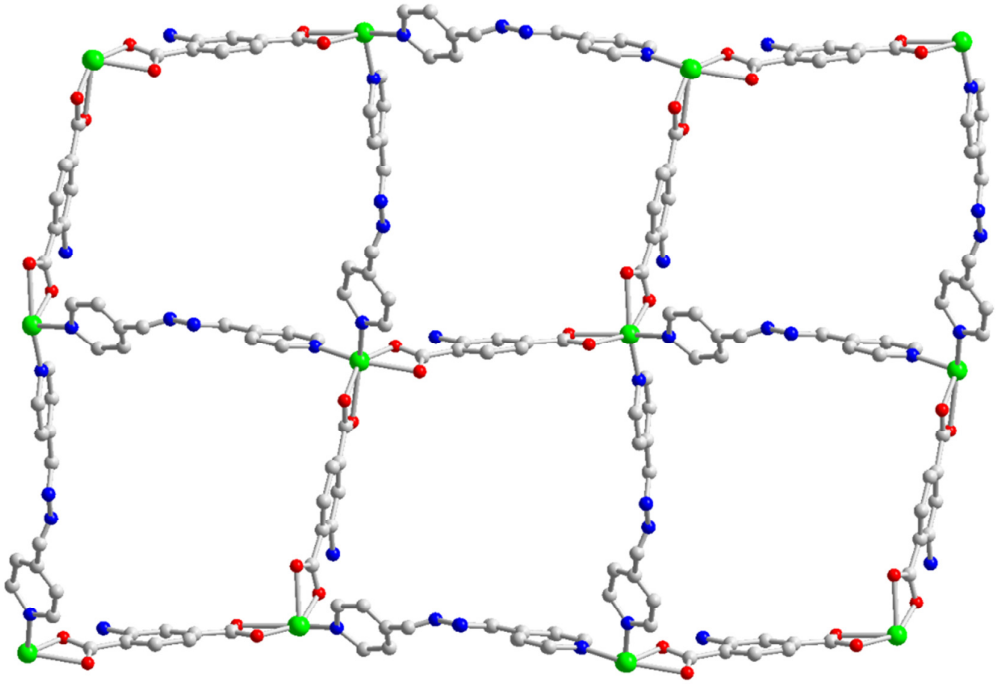

Figure S12. Illustration of 2d sheet like network found in compound **2** along the *b*-axis. Color code; same as in Figure S2.

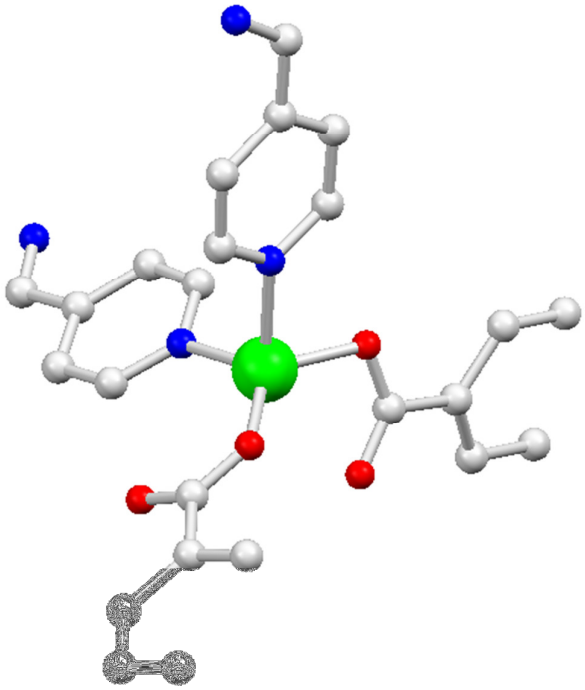

Figure S13. Asymmetric unit of **3**. Color code: carbon (light gray), nitrogen (blue), oxygen (red) and zinc (green). (Hydrogens are omitted for clarity).

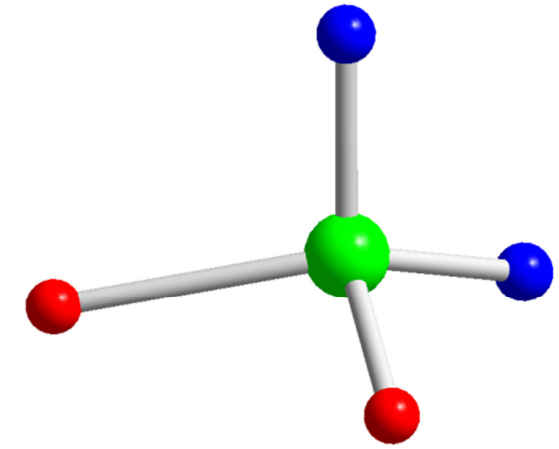

Figure S14. A distorted tetrahedral geometry of Zn(II) ion found in compound **3**. Color code; same as in Figure S12.

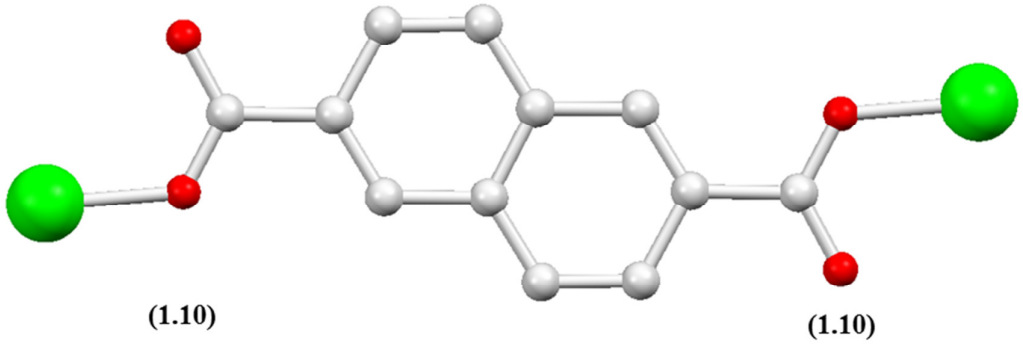

Figure S15. Bridging Mode of NDC found in compound **3** (Harris Notation). Color code; same as in Figure S12.

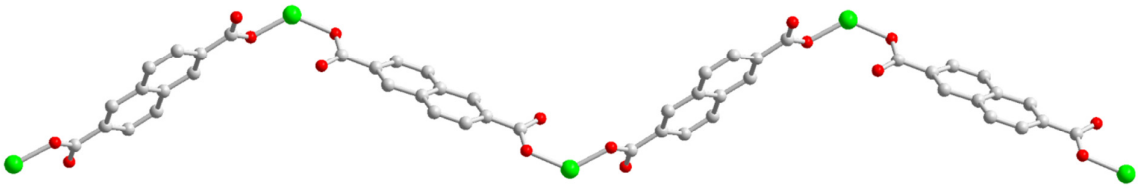

Figure S16. Illustration of 1D zig-zag chain along the *c*-axis. Color code; same as in Figure S12.

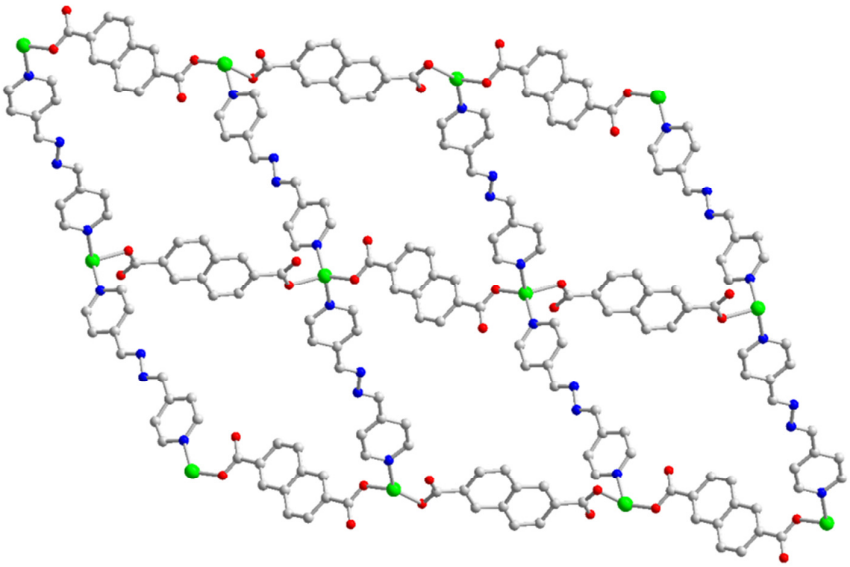

Figure S17. Illustration of 2d sheet like network found in compound **3** along the *b*-axis. Color code; same as in Figure S7.

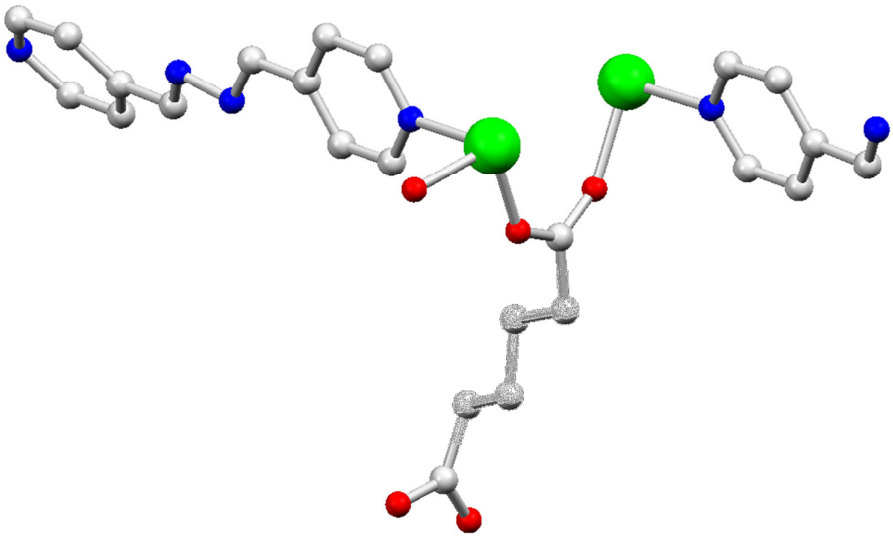

Figure S18. Asymmetric unit of compound **4**. Color code: carbon (light gray), nitrogen (blue), oxygen (red) and zinc (green). (Hydrogens, methanol, perchlorate molecules are omitted for clarity).

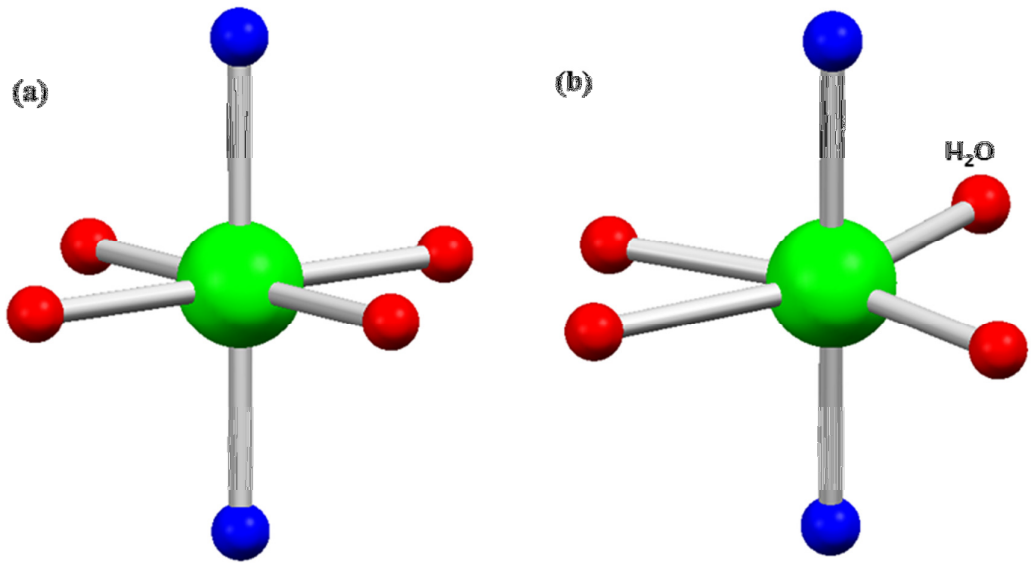

Figure S19. (a) A octahedral geometry of Zn(II) ion (b) distorted octahedral geometry of Zn (II) ion found in compound **4**. (b) Color code; same as in Figure S17.

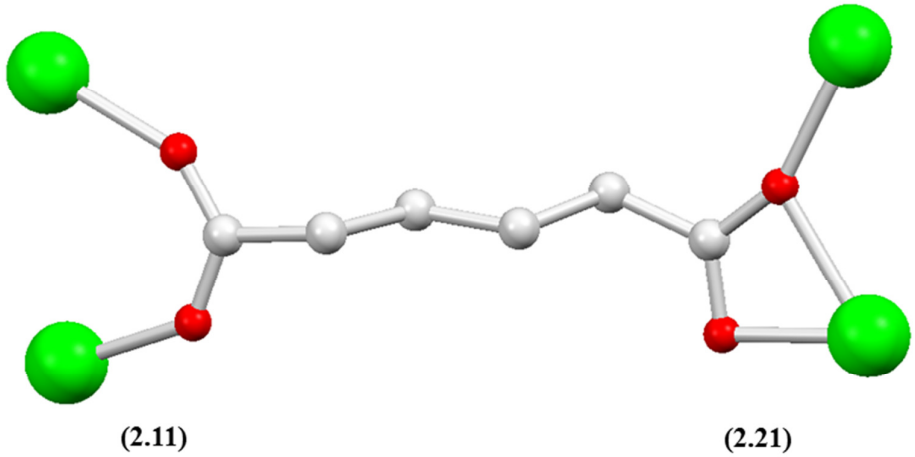

Figure S20. Bridging Mode of ADPA found in compound **4** (Harris Notation). Color code; same as in Figure S17.

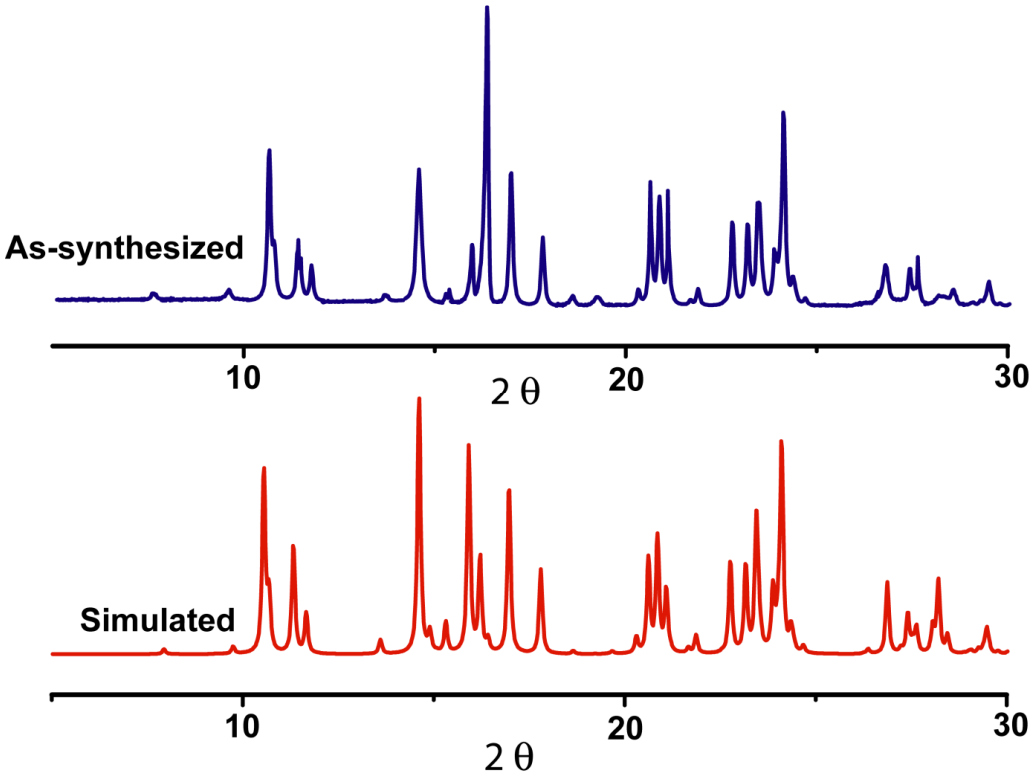

Figure S21. PXRD patterns of compound **1**.

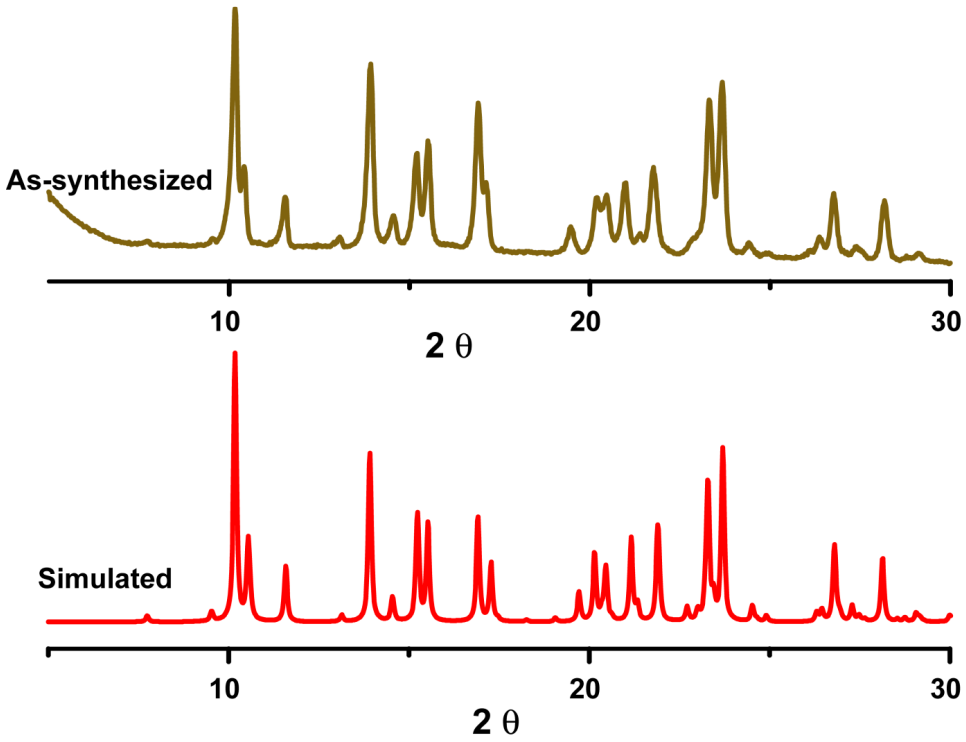

Figure S22. Pxrd patterns of compound **2**.

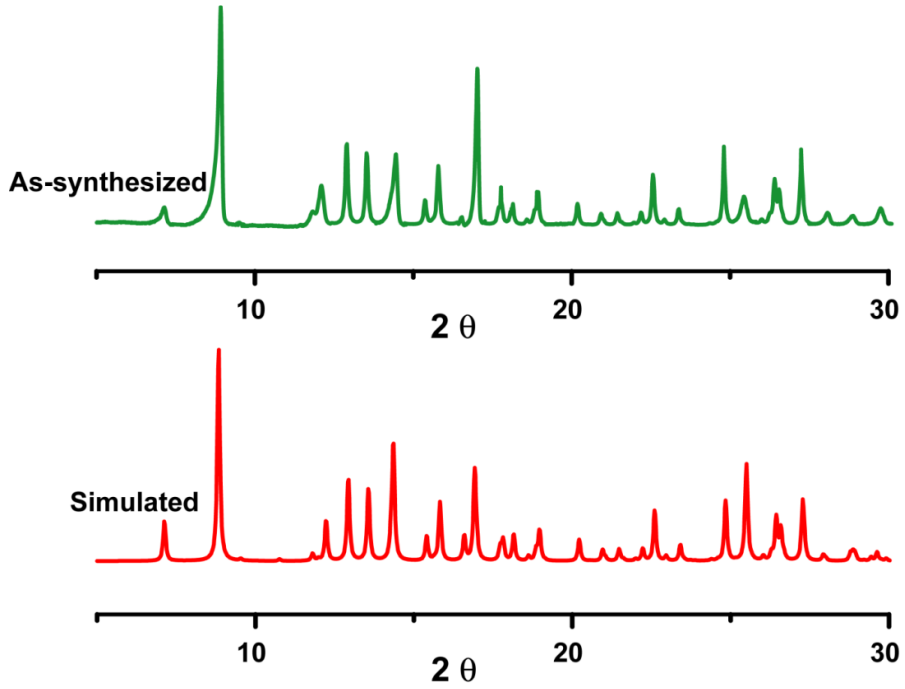

Figure S23. PXRD patterns of compound **3**.

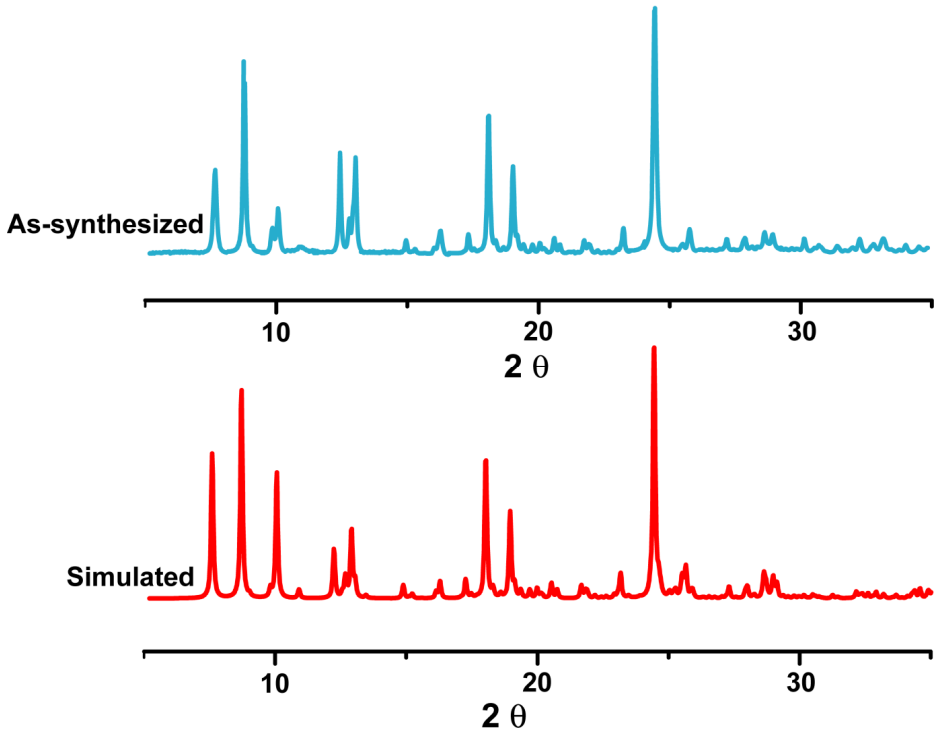

Figure S24. PXRD patterns of compound **4**.

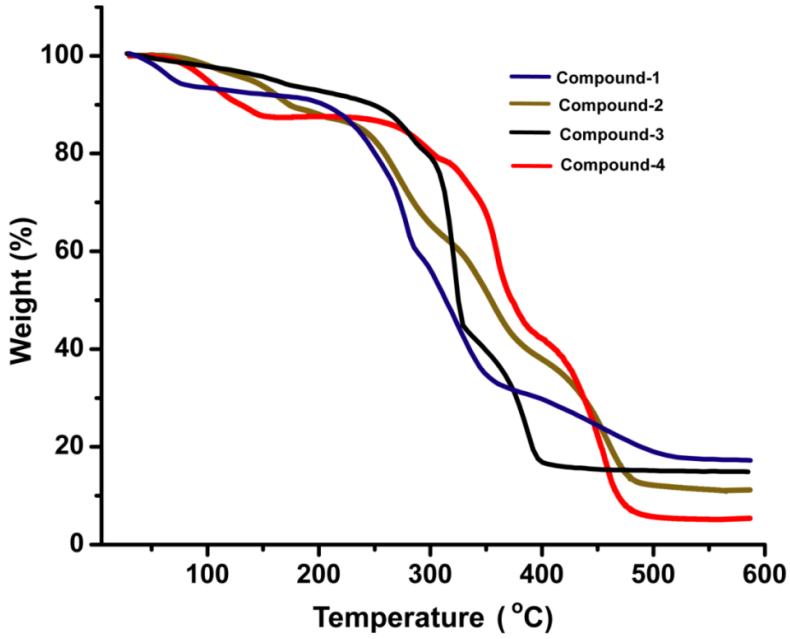

Figure S25. TGA graph of Compounds **1-4.**

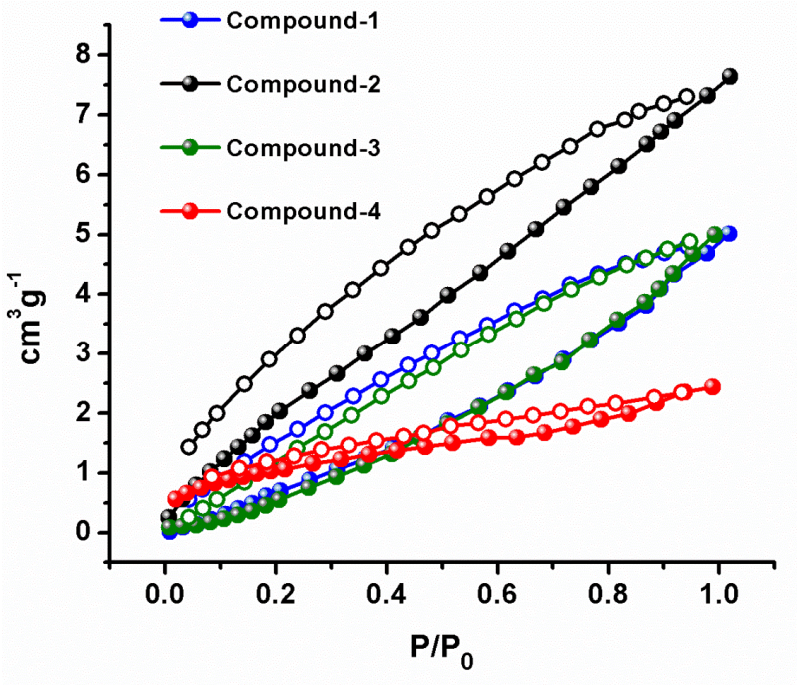

Figure S26. N_2 gas adsorption isotherms of compounds **1**-**4** mesured at 77 K

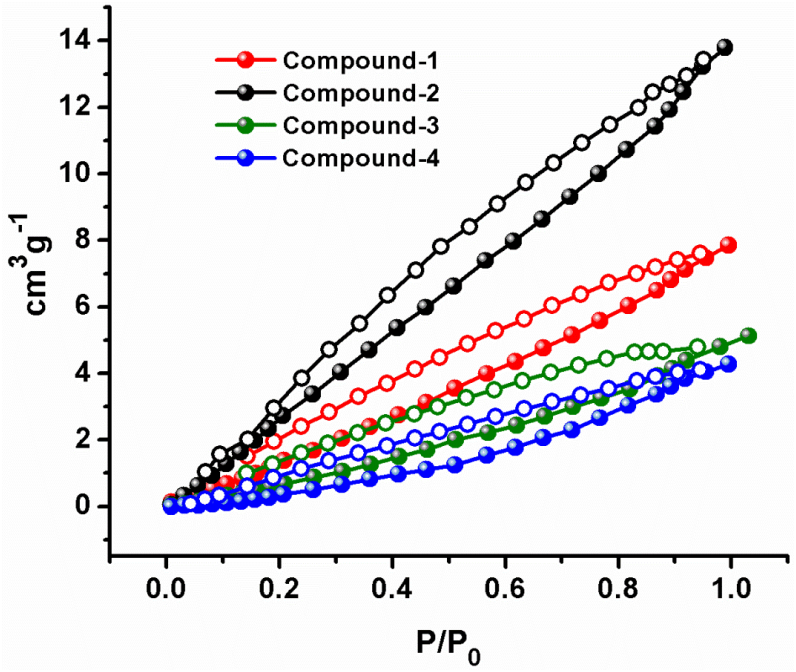

Figure S27. CH_4 gas adsorption isotherms of compounds **1**-**4** mesured at 195 K

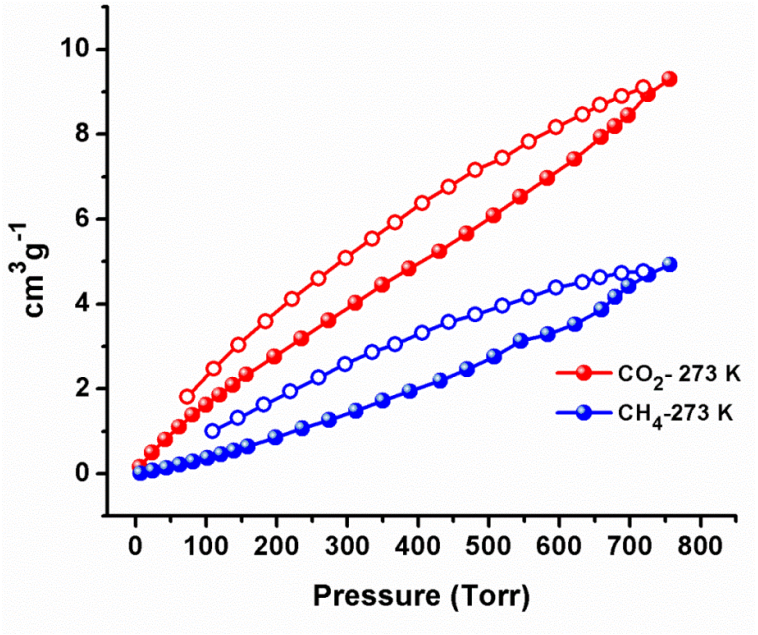

Figure S28. Gas adsorption isotherms of compounds **3** mesured at 273 K

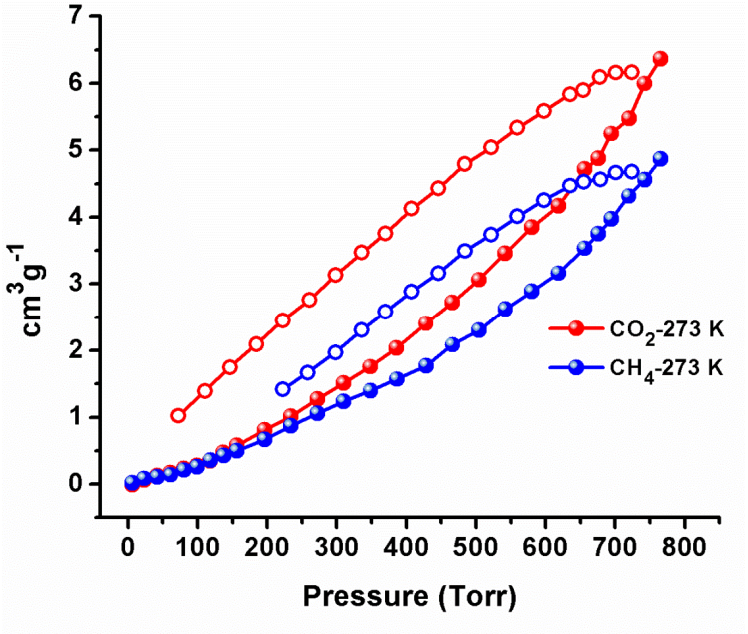

Figure S29. Gas adsorption isotherms of compounds **4** mesured at 273 K.

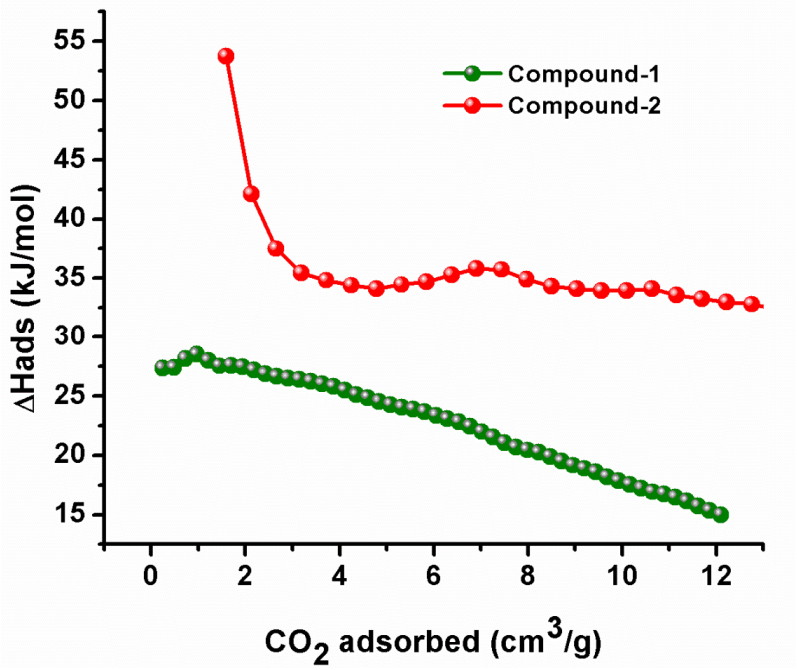

Figure S30. Isosteric heats (Q_{st}) of CO_2 adsorption are calculated based on the adsorption data collected at 273 K and 298 K by using Clapeyron method.

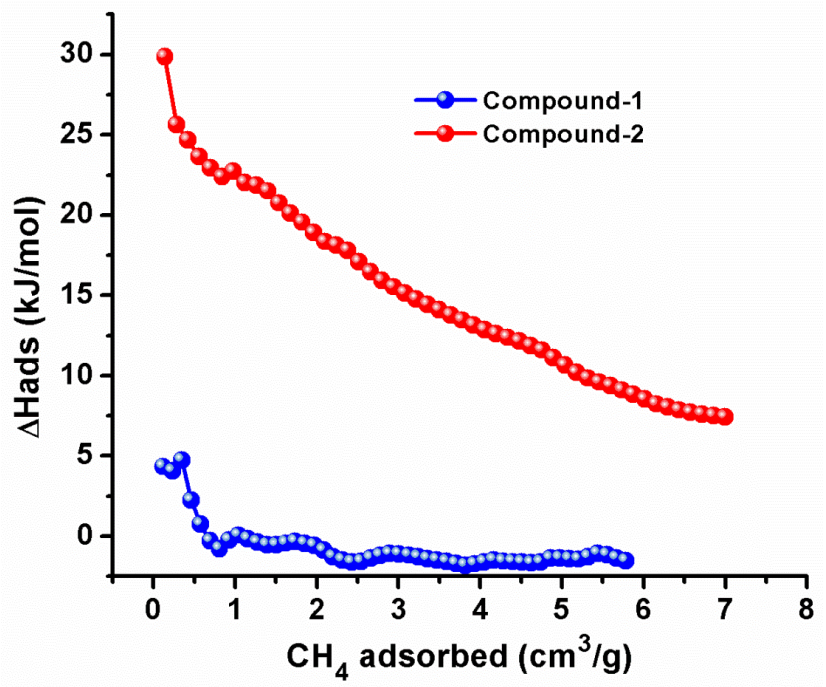

Figure S31. Isosteric heats (Q_{st}) of CH_4 adsorption are calculated based on the adsorption data collected at 273 K and 298 K by using Clapeyron method.

Table S1. Selected bond lengths and bond angles of compound **1**

Bond lengths		**Bond Angles**	
Zn1-O1	2.0089(2)	O1-Zn1-O2	57.44(5)
Zn1-O2	2.505(1)	O1-Zn1-O4	108.21(6)
Zn1-O4	1.952(1)	O2-Zn1-O4	91.32(5)
Zn1-N11	2.084(1)	O1-Zn1-N11	95.74(6)
Zn1-N14	2.017(1)	O1-Zn1-N14	109.25(6)
		O2-Zn1-N11	153.16(5)
		O2-Zn1-N14	86.43(5)
		O4-Zn1-N11	97.19(6)
		O4-Zn1-N14	133.55(6)
		N14-Zn1-N11	105.32(6)

Table S2. Selected bond lengths and bond angles of compound **2**

Bond lengths		**Bond Angles**	
Zn1-O1	2.013(5)	N1-Zn1-O1	106.3(2)
Zn1-O2	2.427(4)	N1-Zn1-O2	89.9(1)
Zn1-N2	2.085(4)	N1-Zn1-N2	101.8(2)
Zn1-O4	2.058(5)	N1-Zn1-O4	96.1(2)
Zn1-O3	2.324(4)	N1-Zn1-O3	154.8(2)
Zn1-N1	2.077(4)	N1-Zn1-O3	154.8(2)
		O1-Zn1-O2	58.2(2)
		O1-Zn1-N2	96.2(2)
		O1-Zn1-O4	145.2(2)
		O1-Zn1-O3	94.7(2)
		O2-Zn1-N2	154.1(2)
		O2-Zn1-O4	96.4(2)
		O2-Zn1-O3	89.4(1)
		N2-Zn1-O4	105.1(2)
		N2-Zn1-O3	89.4(2)
		O4-Zn1-O3	59.0(2)

Table S3. Selected bond lengths and bond angles of compound **3**

Bond lengths		**Bond Angles**	
Zn1-O2	1.920(4)	O2-Zn1-O5	128.3(2)
Zn1-N1	2.059(5)	O2-Zn1-N1	126.0(1)
Zn1-O5	1.991(3)	O2-Zn1-N3	100.4(1)
Zn1-N3	2.091(3)	O5-Zn1-N1	98.0(2)
		O5-Zn1-N3	93.5(2)
		N1-Zn1-N3	103.0(1)

Table S4. Selected bond lengths and bond angles of compound **4**

Bond lengths		**Bond Angles**	
Zn1-O2	2.000(2)	O2-Zn1-O1	100.14(9)
Zn1-O1	2.109(2)	O2-Zn1-N1	90.89(9)
Zn1-N1	2.153(2)	O2-Zn1-O4	163.08(8)
Zn1-O4	2.116(2)	O2-Zn1-O5	103.93(8)
Zn1-O5	2.269(2)	O2-Zn1-N4	90.00(9)
Zn1-N4	2.184(2)	O1-Zn1-N1	88.7(1)
Zn2-O3	2.115	O1-Zn1-O4	96.60(9)
Zn2-N5	2.149	O1-Zn1-O5	155.92(9)
Zn2-O5	2.149	O1-Zn1-N4	90.1(1)
Zn2-O5	2.149	N1-Zn1-O4	91.99(8)
Zn2-O3	2.115	N1-Zn1-O5	90.25(8)
		N1-Zn1-N4	178.61(9)
		O4-Zn1-O5	59.40(7)
		O4-Zn1-N4	87.47(8)
		O5-Zn1-N4	90.58(8)
		O3-Zn2-N5	89.93
		O3-Zn2-O5	87.72
		O3-Zn2-O5	92.28
		O3-Zn2-O3	180.00
		O3-Zn2-N5	90.07
		N5-Zn2-O5	88.90
		N5-Zn2-O5	91.10
		N5-Zn2-O3	90.07
		N5-Zn2-N5	180.00
		O5-Zn2-O5	180.00
		O5-Zn2-O5	180.00
		O5-Zn2-O3	87.72
		O5-Zn2-N5	91.10
		O5-Zn2-O3	92.28
		O5-Zn2-N5	88.90
		O3-Zn2-N5	89.93
		Zn1-O5-Zn2	118.78