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Supporting information

Scheme S1

Figure S1. I.R. spectra of (a) **1**, (b) **2** and (c) **3**.

Figure S2. DTA-TG curves for (a) **1**, (b) **2** and (c) **3**.

Figure S3 (a) Assembly of crystal structures from the transition metal-ptc compounds and **1**; **(b)** The evolving of crystal structures for the transition metal-ptc compounds; **(c)** The metal oxide unit in the transition metal hydroxo ptc complexes.

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Scheme S1

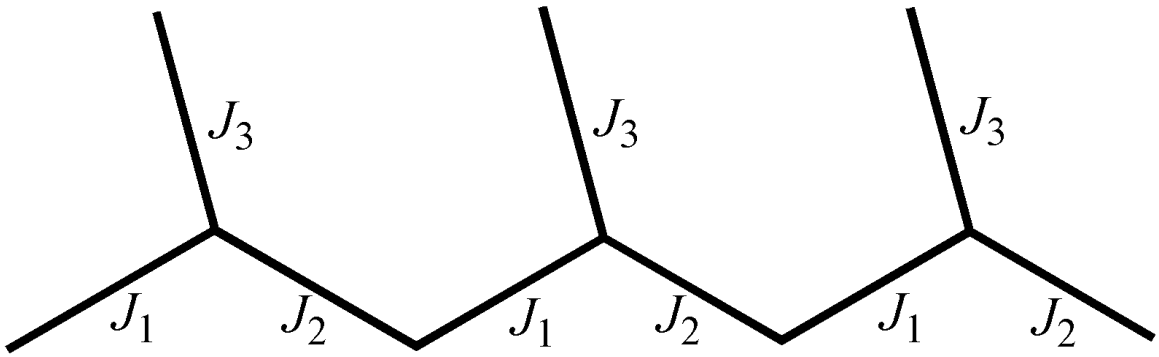

Table S1a. Selected Interatomic Distances (Å) and Bond Angles (deg) for **1**[a]

Mn1–O1	2.291(3)	Mn2–O2	2.140(3)	Mn3–O3	2.123(3)
Mn1–O6	2.258(3)	Mn2–O7	2.331(3)	Mn3–O5$^{\#1}$	2.188(3)
Mn1–O11$^{\#2}$	2.229(3)	Mn2–O12	2.474(4)	Mn3–O18	2.204(3)
Mn1–O12$^{\#2}$	2.458(3)	Mn2–O15	2.226(3)	Mn3–O19	2.140(3)
Mn1–O13	2.215(3)	Mn2–O16	2.369(4)	Mn3–O20	2.195(3)
Mn1–O14	2.208(3)	Mn2–O17	2.143(3)	Mn3–O21	2.194(3)
Mn1–N1	2.214(3)	Mn2–N2	2.299(3)		
O1–Mn1–O6	144.4(1)	O13–Mn1–N1	99.2(1)	O15–Mn2–N2	91.6(1)
O1–Mn1–O11$^{\#2}$	77.5(1)	O14–Mn1–N1	91.8(1)	O16–Mn2–O17	106.2(1)
O1–Mn1–O12$^{\#2}$	132.9(1)	O2–Mn2–O7	94.2(1)	O16–Mn2–N2	118.6(1)
O1–Mn1–O13	99.1(1)	O2–Mn2–O12	128.3(1)	O17–Mn2–N2	98.1(1)
O1–Mn1–O14	91.2(1)	O2–Mn2–O15	88.3(1)	O3–Mn3–O5$^{\#1}$	164.5(1)
O1–Mn1–N1	70.4(1)	O2–Mn2–O16	78.0(1)	O3–Mn3–O18	90.7(1)
O6–Mn1–O11$^{\#2}$	141.0(1)	O2–Mn2–O17	79.9(1)	O3–Mn3–O19	85.8(1)
O6–Mn1–O12$^{\#2}$	85.7(1)	O2–Mn2–N2	162.9(1)	O3–Mn3–O20	101.2(1)
O6–Mn1–O13	86.2(1)	O7–Mn2–O12	133.4(1)	O3–Mn3–O21	97.0(1)
O6–Mn1–O14	90.8(1)	O7–Mn2–O15	80.7(1)	O5$^{\#1}$–Mn3–O18	79.5(1)
O6–Mn1–N1	71.1(1)	O7–Mn2–O16	155.4(1)	O5$^{\#1}$–Mn3–O19	84.3(1)
O11$^{\#2}$–Mn1–O12$^{\#2}$	55.4(1)	O7–Mn2–O17	95.1(1)	O5$^{\#1}$–Mn3–O20	90.8(1)
O11$^{\#2}$–Mn1–O13	86.0(1)	O7–Mn2–N2	69.0(1)	O5$^{\#1}$–Mn3–O21	94.0(1)
O11$^{\#2}$–Mn1–O14	88.4(1)	O12–Mn2–O15	114.2(1)	O18–Mn3–O19	100.9(1)
O11$^{\#2}$–Mn1–N1	147.9(1)	O12–Mn2–O16	65.0(1)	O18–Mn3–O20	164.4(1)
O12$^{\#2}$–Mn1–O13	78.6(1)	O12–Mn2–O17	77.5(1)	O18–Mn3–O21	84.3(1)
O12$^{\#2}$–Mn1–O14	88.5(1)	O12–Mn2–N2	66.9(1)	O19–Mn3–O20	90.1(1)
O12$^{\#2}$–Mn1–N1	156.8(1)	O15–Mn2–O16	75.9(1)	O19–Mn3–O21	174.2(1)
O13–Mn1–O14	167.0(1)	O15–Mn2–O17	167.2(1)	O20–Mn3–O21	84.4(1)

Symmetry transformations used to generate equivalent atoms: #1 = x–1/2, –y+1/2, z–1/2; #2 = x+1/2, –y+1/2, z+1/2

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Table S1b. Selected hydrogen bond for **1**[a]

D–H···A	d(D–H)	d(H···A)	∠DHA	d(D···A)
O13–H13A···O8$^{\#3}$	0.85	1.91	154	2.699
O13–H13B···O4$^{\#4}$	0.74	2.18	158	2.878
O14–H14A···O9$^{\#5}$	0.82	1.95	171	2.756
O14–H14B···O3$^{\#6}$	0.76	2.24	163	2.977
O15–H15A···O9$^{\#5}$	0.81	2.00	167	2.796
O15–H15B···O5$^{\#7}$	0.86	2.08	150	2.860
O16–H16A···O12	0.82	2.15	115	2.604
O16–H16A···O13$^{\#1}$	0.82	2.31	149	3.045
O16–H16B···O10$^{\#5}$	0.85	1.93	166	2.754
O17–H17A···O10$^{\#3}$	0.86	2.09	153	2.879
O17–H17B···O4$^{\#8}$	0.82	2.01	151	2.753
O18–H18A···O1$^{\#9}$	0.77	2.14	152	2.842
O18–H18B···O7$^{\#9}$	0.81	2.06	163	2.843
O19–H19A···O11$^{\#3}$	0.79	1.97	166	2.741
O19–H19A···O1$^{\#10}$	0.79	2.59	118	3.039
O19–H19B···O7$^{\#10}$	0.85	2.06	168	2.897
O20–H20A···O6$^{\#1}$	0.77	2.21	136	2.813
O20–H20B···O10$^{\#3}$	0.78	2.08	167	2.842
O21–H21A···O16	0.78	2.12	165	2.884
O21–H21B···O8$^{\#9}$	0.75	2.13	157	2.833

Symmetry transformations used to generate equivalent atoms: #1 = x–1/2, –y+1/2, z–1/2; #2 = x+1/2, –y+1/2,z+1/2; #3 = x, –y, z+1/2; #4 = x+1/2, y–1/2, z; #5 = x, –y+1, z+1/2; #6 = x+1/2, y+1/2, z; #7 = x, –y+1, z–1/2; #8 = x, –y, z–1/2; #9 = x–1/2, y+1/2, z; #10 = x–1/2, y–1/2, z

Table S2. Selected Interatomic Distances (Å) and Bond Angles (deg) for **2**[a]

Co1–O1	2.206(2)	Co1–N	2.017(2)	Co2–O4$^{\#4}$	2.012(2)
Co1–O1$^{\#1}$	2.206(2)	Co1–N$^{\#1}$	2.017(2)	Co2–O5	2.124(2)
Co1–O6	2.103(2)	Co2–O1$^{\#2}$	2.186(2)	Co2–O7	2.158(2)
Co1–O6$^{\#1}$	2.103(2)	Co2–O3$^{\#3}$	2.083(2)	Co2–O7$^{\#5}$	2.188(2)
O1–Co1–O1$^{\#1}$	101.5(1)	O6–Co1–O6$^{\#1}$	84.8(1)	O3$^{\#3}$–Co2–O4$^{\#4}$	84.1(1)
O1–Co1–O6	152.0(1)	O6–Co1–N	76.7(1)	O3$^{\#3}$–Co2–O5	94.3(1)
O1–Co1–O6$^{\#1}$	93.0(1)	O6–Co1–N$^{\#1}$	95.5(1)	O3$^{\#3}$–Co2–O7	92.1(1)
O1–Co1–N	75.7(1)	O6$^{\#1}$–Co1–N	95.5(1)	O3$^{\#3}$–Co2–O7$^{\#5}$	90.0(1)
O1–Co1–N$^{\#1}$	111.2(1)	O6$^{\#1}$–Co1–N$^{\#1}$	76.7(1)	O4$^{\#4}$–Co2–O5	89.4(1)
O1$^{\#1}$–Co1–O6	93.0(1)	O1$^{\#2}$–Co2–O3$^{\#3}$	173.0(1)	O4$^{\#4}$–Co2–O7	176.1(1)
O1$^{\#1}$–Co1–O6$^{\#1}$	152.0(1)	O1$^{\#2}$–Co2–O4$^{\#4}$	93.5(1)	O4$^{\#4}$–Co2–O7$^{\#5}$	91.0(1)
O1$^{\#1}$–Co1–N	111.2(1)	O1$^{\#2}$–Co2–O5	92.2(1)	O5–Co2–O7	89.9(1)
O1$^{\#1}$–Co1–N$^{\#1}$	75.7(1)	O1$^{\#2}$–Co2–O7	90.4(1)	O5–Co2–O7$^{\#5}$	94.3(1)
O1–Co1–O6	101.5(1)	O1$^{\#2}$–Co2–O7$^{\#5}$	83.5(1)	O7–Co2–O7$^{\#5}$	90.0(1)

Hydrogen bonding contacts

D–H···A	d(D–H)	d(H···A)	∠DHA	d(D···A)
O7–H7A···O2$^{\#2}$	0.80	1.89	157	2.643
O7–H7B···O6	0.83	1.83	150	2.575

Symmetry transformations used to generate equivalent atoms: #1 = –x, y, –z+3/2; #2 = –x, y+1, –z+3/2; #3 = x–1/2, –y+3/2, –z+2; #4 = –x, –y+2, –z+2; #5 = –x–1/2, y+1/2, z; #6 = –x, y–1, –z+3/2; #7 = x+1/2, –y+3/2, –z+2; #8 = –x–1/2, y–1/2, z

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Table S3. Selected Interatomic Distances (Å) and Bond Angles (deg) for **3**[a]

Co1–O1	2.104(2)	Co1–O7	2.152(3)	Co2–O9	2.140(2)
Co1–O3$^{\#1}$	2.329(2)	Co1–N1	2.049(2)	Co2–O9$^{\#5}$	2.140(2)
Co1–O3$^{\#2}$	2.046(2)	Co2–O8	2.060(2)	Co2–ON	2.130(1)
Co1–O6	2.113(2)	Co2–O8$^{\#5}$	2.060(2)	Co2–ON$^{\#5}$	2.130(1)
O1–Co1–O3$^{\#1}$	84.3(1)	O3$^{\#2}$–Co1–O7	93.9(1)	O8$^{\#5}$–Co2–O9	90.3(1)
O1–Co1–O3$^{\#2}$	105.3(1)	O3$^{\#2}$–Co1–N1	178.4(1)	O8$^{\#5}$–Co2–O9$^{\#5}$	89.7(1)
O1–Co1–O6	149.4(1)	O6–Co1–O7	97.4(1)	O8$^{\#5}$–Co2–N2	89.0(1)
O1–Co1–O7	90.5(1)	O6–Co1–N1	75.1(1)	O8$^{\#5}$–Co2–N2$^{\#5}$	91.0(1)
O1–Co1–N1	75.7(1)	O7–Co1–N1	87.3(1)	O9–Co2–O9$^{\#5}$	180.0(1)
O3$^{\#1}$–Co1–O3$^{\#2}$	77.9(1)	O8–Co2–O8$^{\#5}$	180.0	O9–Co2–N2	90.8(1)
O3$^{\#1}$–Co1–O6	92.1(1)	O8–Co2–O9	89.7(1)	O9–Co2–N2$^{\#5}$	89.2(1)
O3$^{\#1}$–Co1–O7	168.7(1)	O8–Co2–O9$^{\#5}$	90.3(1)	O9$^{\#5}$–Co2–N2	89.2(1)
O3$^{\#1}$–Co1–N1	101.1(1)	O8–Co2–N2	91.0(1)	O9$^{\#5}$–Co2–N2$^{\#5}$	90.8(1)
O3$^{\#2}$–Co1–O6	103.6(1)	O8–Co2–N2$^{\#5}$	89.0(1)	N2–Co2–N2$^{\#5}$	180.0(1)

Hydrogen bonding contacts

D–H···A	d(D–H)	d(H···A)	∠DHA	d(D···A)
O7–H7A···O4$^{\#8}$	0.85	2.03	166	2.865
O7–H7B···O3$^{\#2}$	0.86	2.21	180	3.069
O7–H7B···O4$^{\#2}$	0.86	2.36	122	2.902
O8–H8A···O6$^{\#8}$	0.85	1.83	172	2.671
O8–H8B···O1$^{\#9}$	0.85	1.85	168	2.681
O9–H9C···O5$^{\#10}$	0.85	1.94	173	2.780
O9–H9B···O2$^{\#9}$	0.85	1.96	172	2.800

Symmetry transformations used to generate equivalent atoms: #1 = –x+2, –y+1, –z+2; #2 = x, y+1, z; #3 = x, y–1, z; #4 = –x+2, –y+2, –z+2; #5 = –x+1, –y, –z+1; #6 = –x, –y+1, –z+1; #7 = x–1, y+1, z; #8 = –x+1, –y+1, –z+2; #9 = x–1, y–1, z; #10 = x, y–1, z-1

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Figure S1. I.R spectra of (a) **1**, (b) **2** and (c) **3**.

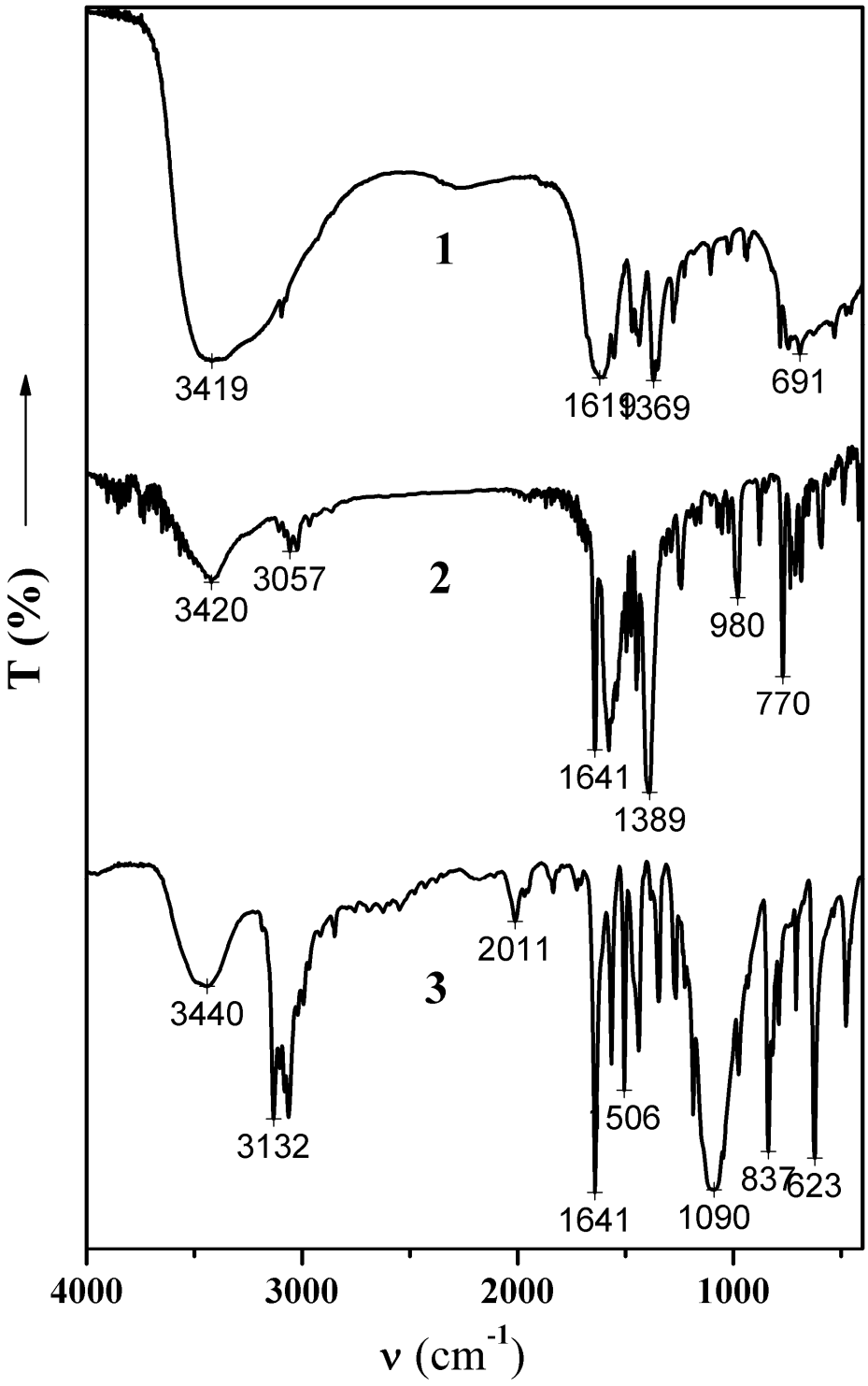

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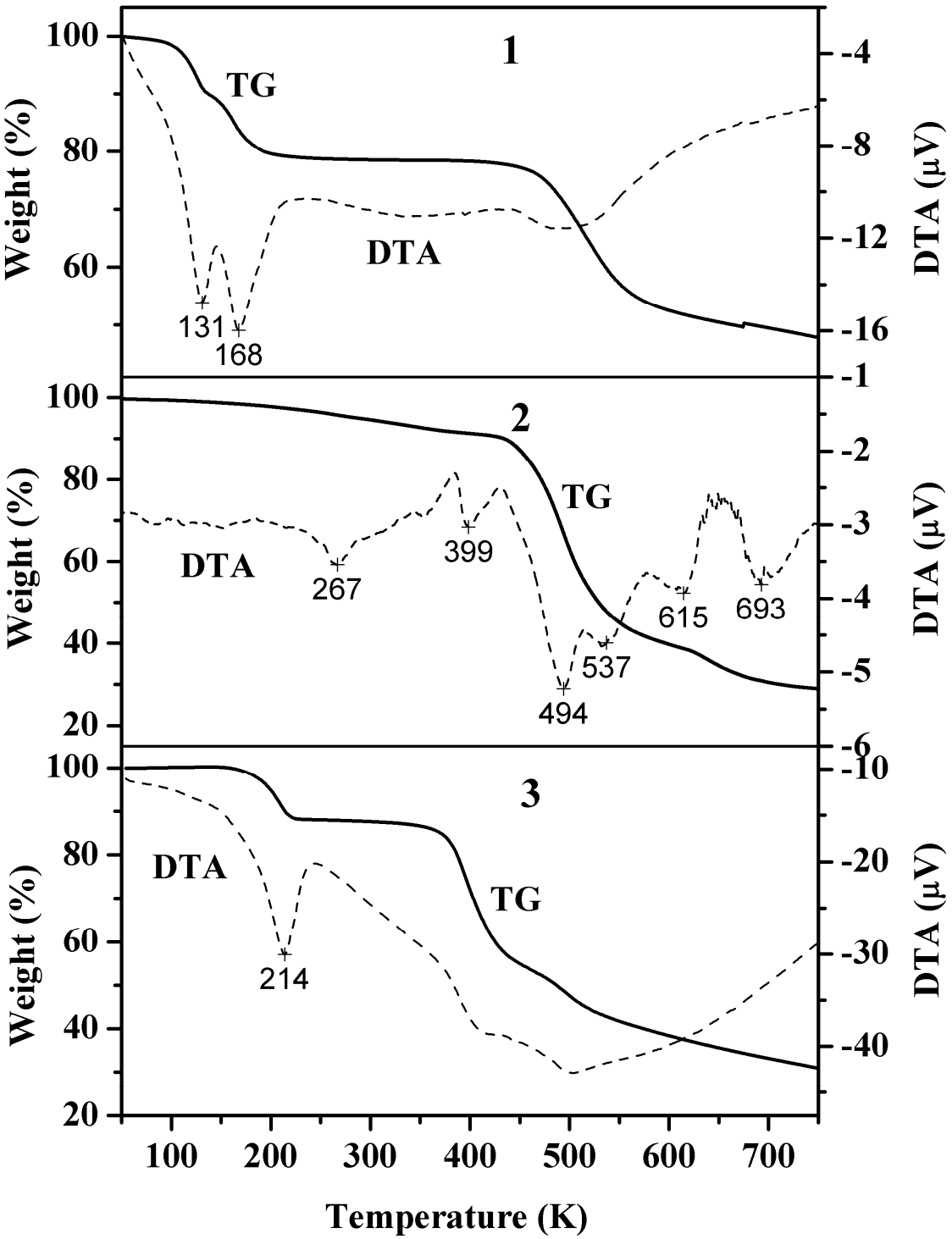
Figure S2. DTA-TG curves for (a) **1**, (b) **2** and (c) **3**.



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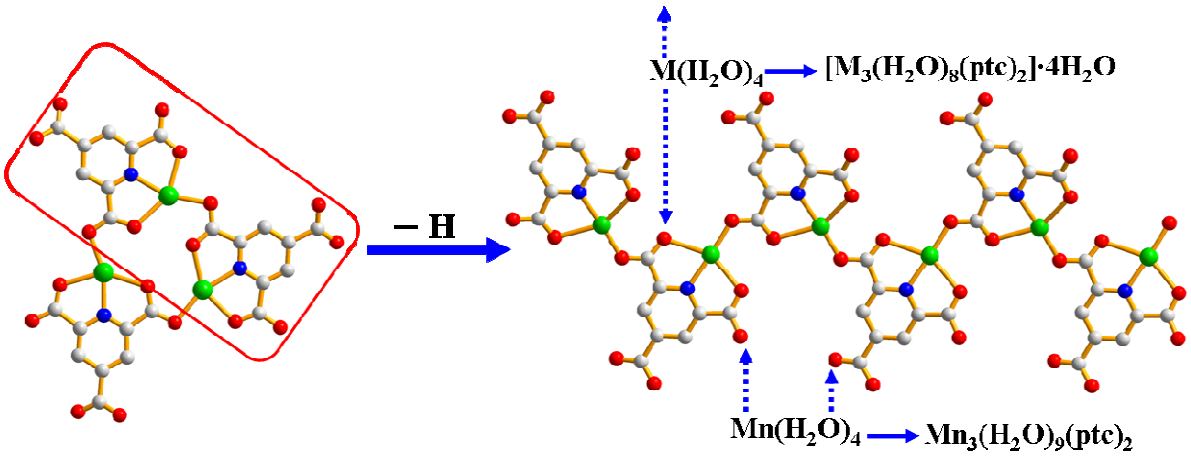

Figure S3a. Assembly of crystal structures from the transition metal-ptc compounds and **1.**

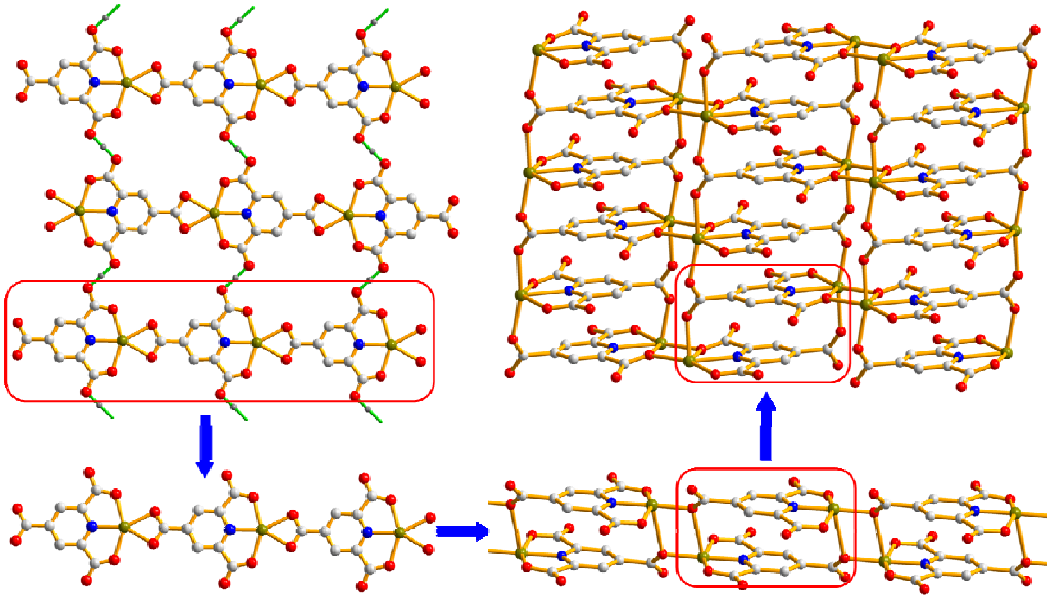

Figure S3b. The evolving of crystal structures for the transition metal-ptc compounds.

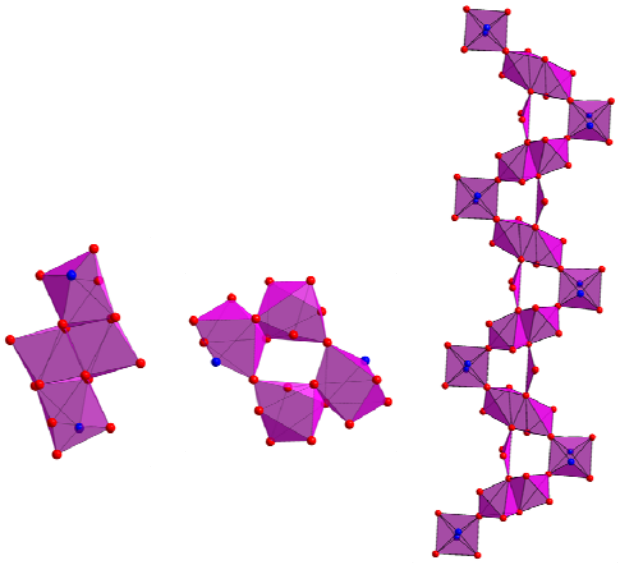

Figure S3c. The metal oxide unit in the transition metal hydroxo ptc complexes.