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Roles of Temperature, Solvent, M/L ratios and Anion in Preparing the Complexes Containing Himta Ligand

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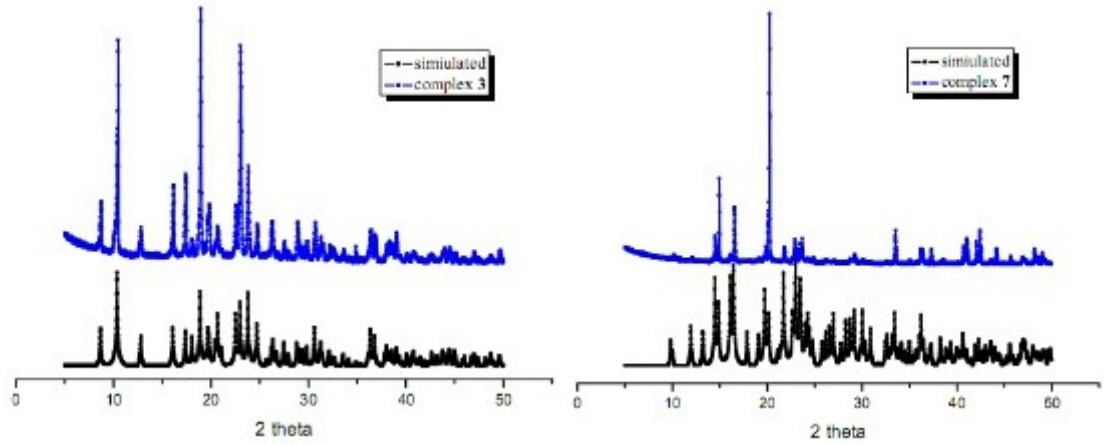

(a) (b)

Figure S1. Powder X-ray diffraction (PXRD) patterns of **3** and **7**: (a) simulated PXRD pattern from the single crystal structure of **3** (black), observed PXRD pattern of **3** at room temperature (blue). (2) simulated PXRD pattern from the single crystal of **7** (black), observed PXRD pattern of **7** at room temperature (blue).

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Electronic supplementary information (ESI) available: The X-ray crystallographic files in CIF format. CCDC reference numbers 1437785-1437793 are for **1~9**, respectively.

Table S1. Selected Bond Lengths (Å) and Angles (deg) for complexes 1~5

Complex **1**					
Cu(1)-O(2)#1	1.957(3)	O(2)#2-Cu(1)-N(1)#3	88.91(15)	Cu(1)-N(1)#3	1.972(4)
Cu(1)-O(2)#2	1.957(3)	O(2)#1-Cu(1)-N(1)	88.91(15)	Cu(1)-N(1)	1.972(4)
O(2)#1-Cu(1)-O(2)#2	180	O(2)#2-Cu(1)-N(1)	91.09(15)	N(1)#3-Cu(1)-N(1)	180
O(2)#1-Cu(1)-N(1)#3	91.09(15)				
Complex **2**					
Co(1)-O(1)#3	2.080(3)	Co(1)-O(1)#4	2.080(3)	Co(1)-O(2)#5	2.131(3)
Co(1)-O(2)	2.131(3)	Co(1)-N(2)#6	2.173(3)	Co(1)-N(2)#7	2.173(3)
O(1)#3-Co(1)-O(1)#4	180	O(1)#3-Co(1)-O(2)#5	90.62(12)	O(1)#4-Co(1)-O(2)#5	89.38(1)
N(2)#6-Co(1)-N(2)#7	180	O(2)-Co(1)-N(2)#7	86.17(13)	O(2)#5-Co(1)-N(2)#7	93.83(1)
O(1)#4-Co(1)-N(2)#7	94.36(13)	O(1)#3-Co(1)-N(2)#7	85.64(12)	O(2)-Co(1)-N(2)#6	93.83(1)
Co(1)-O(1)#3	2.080(3)	Co(1)-O(1)#4	2.080(3)	Co(1)-O(2)#5	2.131(3)
Complex **3**					
Mn(1)-N(5)#7	2.282(2)	Mn(1)-O(2)#3	2.1753(19)	Mn(1)-O(2)#4	2.175(3)
Mn(1)-O(1)#5	2.2062(19)	Mn(1)-O(1)	2.2062(19)	Mn(1)-N(5)#6	2.282(2)
O(2)#3-Mn(1)-O(2)#4	180	O(2)#3-Mn(1)-O(1)#5	89.49(7)	O(2)#4-Mn(1)-O(1)#5	90.51(7)
N(5)#6-Mn(1)-N(5)#7	180	O(1)-Mn(1)-N(5)#7	94.56(8)	O(1)#5-Mn(1)-N(5)#7	85.44(8)
O(2)#4-Mn(1)-N(5)#7	85.76(8)	O(2)#3-Mn(1)-N(5)#7	94.24(8)	O(1)-Mn(1)-N(5)#6	85.44(8)
Complex **4**					
Cd(1)-N(2)#7	2.325(3)	Cd(1)-O(2)#3	2.307(3)	Cd(1)-O(2)#4	2.307(3)
Cd(1)-O(1)#5	2.325(3)	Cd(1)-O(1)#6	2.325(3)	Cd(1)-N(2)	2.325(3)
O(1)#5-Cd(1)-N(2)	95.62(11)	O(2)#3-Cd(1)-O(2)#4	180	O(2)#3-Cd(1)-O(1)#5	88.37(1)
O(2)#4-Cd(1)-O(1)#5	91.63(10)	O(2)#3-Cd(1)-O(1)#6	91.63(10)	O(2)#4-Cd(1)-O(1)#6	88.37(1)
O(1)#5-Cd(1)-O(1)#6	180	N(2)-Cd(1)-N(2)#7	180	O(1)#6-Cd(1)-N(2)#7	95.62(1)
Complex **5**					
Pb(1)-O(1)#1	2.441(5)	O(1)#1-Pb(1)-O(1)	78.2(2)	O(1)#4-Pb(1)-O(2)#1	112.76(16)
Pb(1)-O(1)	2.441(5)	O(1)#1-Pb(1)-N(1)#2	79.2(2)	O(1)#5-Pb(1)-O(2)#1	72.60(16)
Pb(1)-N(1)#2	2.656(7)	O(1)-Pb(1)-N(1)#2	79.4(2)	O(1)#1-Pb(1)-O(2)	126.02(16)
Pb(1)-N(1)#3	2.656(7)	O(1)#1-Pb(1)-N(1)#3	79.4(2)	N(1)#2-Pb(1)-O(2)	87.4(2)

Pb(1)-O(1)#4	2.762(5)	N(1)#3-Pb(1)-O(2)	91.2(2)	O(1)#4-Pb(1)-O(2)	72.60(17)
Pb(1)-O(1)#5	2.762(5)	O(1)#5-Pb(1)-O(2)	112.76(16)	O(3)#1-Pb(1)-O(2)	173.9(2)
Pb(1)-O(2)#1	2.861(6)	N(1)#3-Pb(1)-O(1)#5	127.8(2)	N(1)#2-Pb(1)-O(1)#5	77.54(18)
Pb(1)-O(2)	2.861(6)	O(1)#4-Pb(1)-O(1)#5	67.7(2)	O(1)-Pb(1)-O(1)#5	150.6(3)
O(1)-Pb(1)-N(1)#3	79.2(2)	O(1)#1-Pb(1)-O(2)#1	47.91(15)	O(1)#1-Pb(1)-O(1)#5	114.73(19)
N(1)#2-Pb(1)-N(1)#3	152.3(3)	O(1)-Pb(1)-O(2)#1	126.02(16)	N(1)#3-Pb(1)-O(1)#4	77.54(18)
O(1)#1-Pb(1)-O(1)#4	150.6(3)	N(1)#2-Pb(1)-O(2)#1	91.2(2)	N(1)#2-Pb(1)-O(1)#4	127.8(2)
O(1)-Pb(1)-O(2)	47.91(15)	N(1)#3-Pb(1)-O(2)#1	87.4(2)	O(1)-Pb(1)-O(1)#4	114.73(19)

Symmetry transformations used to generate equivalent atoms:

For **1**: #1 -x+1,y+1/2,-z+1/2, #2 x,-y+1/2,z+1/2, #3 -x+1,-y+1,-z+1, #4 -x+1,y-1/2,-z+1/2

For **2**: #1, x+1,y,z; #2, -x+1,y+1/2,-z+1/2; #3 ,-x+2,-y,-z+1; #4, x-1,y,z; #5, -x+1,-y,-z+1; #6, x,-y+1/2,z+1/2; #7, -x+1,y-1/2,-z+1/2.

For **3**: #1, -x+2,y+1/2,-z+1/2; #2, x-1,y,z; #3, -x+1,-y,-z; #4, x+1,y,z; #5, -x+2,-y,-z; #6, -x+2,y-1/2,-z+1/2; #7, x,-y+1/2,z-1/2.

For **4**: #1, -x+1,y+1/2,-z+1/2; #2, -x,y+1/2,-z+1/2; #3,-x+1,y-1/2,-z+1/2; #4, x,-y+1/2,z+1/2; #5, -x,y-1/2,-z+1/2; #6, x+1,-y+1/2,z+1/2; #7, -x+1,-y,-z+1.

For **5**: #1, -x+3/2,-y+3/2,z; #2, -x+1,y-1/2,-z+3/2; #3, x+1/2,-y+2,-z+3/2; #4, -x+3/2,y,z+1/2; #5, x,-y+3/2,z+1/2; #6, -x+3/2,y,z-1/2; #7, x-1/2,-y+2,-z+3/2.

Table S2. Selected Bond Lengths (Å) and Angles (deg) for complexes 6~9

Complex **6**					
Co(1)-O(3)	2.097(2)	O(4)#1-Co(1)-O(4)	180	N(2)-Co(1)-N(2)#1	180
Co(1)-O(3)#1	2.097(2)	O(3)-Co(1)-N(2)	90.29(9)	O(4)-Co(1)-N(2)#1	88.58(9)
Co(1)-O(4)#1	2.119(2)	O(3)#1-Co(1)-N(2)	89.71(9)	O(4)#1-Co(1)-N(2)#1	91.42(9)
Co(1)-O(4)	2.119(2)	O(4)#1-Co(1)-N(2)	88.58(9)	O(3)#1-Co(1)-N(2)#1	90.29(9)
Co(1)-N(2)	2.148(2)	O(4)-Co(1)-N(2)	91.42(9)	O(3)-Co(1)-N(2)#1	89.71(9)
Co(1)-N(2)#1	2.148(2)	O(3)#1-Co(1)-O(4)#1	92.41(9)	O(3)-Co(1)-O(4)	92.41(9)
Complex **7**					
Mn(1)-O(7)	2.169(2)	O(5)#1-Mn(1)-O(5)	180	O(7)#1-Mn(1)-O(5)	86.70(9)
Mn(1)-O(7)#1	2.169(2)	O(7)-Mn(1)-N(1)	90.28(9)	O(7)-Mn(1)-O(5)	93.30(9)
Mn(1)-O(5)#1	2.194(2)	O(7)#1-Mn(1)-N(1)	89.72(9)	N(1)-Mn(1)-N(1)#1	180
Mn(1)-O(5)	2.194(2)	O(5)#1-Mn(1)-N(1)	88.89(8)	O(7)#1-Mn(1)-O(5)#1	93.30(9)
Mn(1)-N(1)	2.258(2)	O(5)-Mn(1)-N(1)	91.11(8)	O(5)-Mn(1)-N(1)#1	88.89(8)
Mn(1)-N(1)#1	2.258(2)	O(7)-Mn(1)-N(1)#1	89.72(9)	O(7)-Mn(1)-O(5)#1	86.70(9)
O(7)-Mn(1)-O(7)#1	180	O(7)#1-Mn(1)-N(1)#1	90.28(9)	O(5)#1-Mn(1)-N(1)#1	91.11(8)
Complex **8**					
Ni(1)-O(2)#1	2.070(2)	O(2)-Ni(1)-O(1)	92.01(10)	O(1)-Ni(1)-N(2)	91.10(10)
Ni(1)-O(2)	2.070(2)	O(1)#1-Ni(1)-O(1)	180	O(2)#1-Ni(1)-O(1)	87.99(10)
Ni(1)-O(1)#1	2.088(2)	O(2)#1-Ni(1)-N(2)#1	90.82(10)	O(2)-Ni(1)-O(1)#1	87.99(10)
Ni(1)-O(1)	2.088(2)	O(2)-Ni(1)-N(2)#1	89.18(10)	O(1)#1-Ni(1)-N(2)	88.90(10)
Ni(1)-N(2)#1	2.094(2)	O(1)#1-Ni(1)-N(2)#1	91.10(10)	O(2)#1-Ni(1)-O(1)#1	92.01(10)
Ni(1)-N(2)	2.094(2)	O(1)-Ni(1)-N(2)#1	88.90(10)	O(2)-Ni(1)-N(2)	90.82(10)
O(2)#1-Ni(1)-O(2)	180	O(2)#1-Ni(1)-N(2)	89.18(10)		
Complex **9**					
Zn(1)-O(4)	2.114(2)	O(4)-Zn(1)-O(3)#1	92.58(9)	O(4)-Zn(1)-N(1)	90.49(10)
Zn(1)-O(4)#1	2.114(2)	O(4)#1-Zn(1)-O(3)#1	87.42(9)	O(3)#1-Zn(1)-O(3)	180
Zn(1)-N(1)#1	2.123(2)	N(1)#1-Zn(1)-O(3)#1	89.03(9)	O(4)#1-Zn(1)-N(1)	89.51(10)

Zn(1)-N(1)	2.123(2)	N(1)-Zn(1)-O(3)#1	90.97(9)	N(1)#1-Zn(1)-N(1)	180
Zn(1)-O(3)#1	2.150(2)	O(4)-Zn(1)-O(3)	87.42(9)	O(4)-Zn(1)-N(1)#1	89.51(10)
Zn(1)-O(3)	2.150(2)	O(4)#1-Zn(1)-O(3)	92.58(9)	N(1)-Zn(1)-O(3)	89.03(9)
O(4)-Zn(1)-O(4)#1	180	N(1)#1-Zn(1)-O(3)	90.97(9)		

Symmetry transformations used to generate equivalent atoms:
For **6**: #1, -x+1,-y,-z+2. For **7**: #1, -x+1,-y+1,-z-1. For **8**: #1 -x,-y+1,-z+1. For **9**: #1, -x+1,-y,-z+2.

Table S3. Hydrogen bond geometries in the crystal structures of complex 1, 6~9.

D-H···A	D-H	d(H···A)	d(D···A)	∠(DHA)
1				
O(4)-H(4A)···O(3)^{c}	0.89	2.23	2.747(19)	116.7
O(4)-H(4B)···N(5)^{b}	0.87	2.12	2.907(8)	149.7
O(5)-H(5C)···O(5)^{d}	0.85	2.55	3.136(16)	127.4
O(5)-H(5D)···N(4)^{a}	0.85	2.62	3.039(9)	111.3
6				
O3-H3W···O9^{b}	1.07(3)	1.60(3)	2.651(3)	169(2)
O3-H3WA···O2^{c}	0.79(3)	1.95(3)	2.740(3)	176(3)
O4-H4W···O1^{d}	0.84(4)	1.94(4)	2.764(3)	171(3)
O4-H4WA···O1^{a}	0.82(4)	1.93(4)	2.728(3)	162(4)
O9-H9W···O2	0.89(4)	1.98(4)	2.847(3)	164(4)
O9-H9WA···N5^{c}	1.02(5)	1.82(5)	2.838(3)	176(4)
O9-H9WA···N4^{c}	1.02(5)	2.59(5)	3.507(4)	149(4)
7				
O5-H5W···O1^{a}	0.81(4)	2.03(4)	2.859(3)	164(4)
O7-H7W···O2^{b}	0.89(4)	1.84(4)	2.737(3)	178(3)
O5-H5WA···O1^{c}	0.79(3)	1.97(4)	2.754(3)	171(3)
O7-H7WA···O9^{d}	0.79(3)	1.88(3)	2.662(3)	170(3)
O9-H9W···N5^{b}	0.82(4)	2.03(4)	2.843(3)	172(4)
O9-H9WA···O2	0.85(4)	2.03(4)	2.859(3)	164(4)
8				
O1-H1···O6^{a}	0.81	2.00	2.730(3)	150.7
O1-H1W···O6^{b}	1.06	1.70	2.758(3)	176.8
O2-H2···O5^{c}	0.80	2.08	2.718(3)	136.6
O2-H2W···O3	0.86(1)	1.85(1)	2.649(4)	154(3)
O3-H3···N5^{d}	0.85(1)	1.99(3)	2.832(4)	170(18)
O3-H3W···O5^{e}	0.85(1)	2.03(6)	2.834(4)	157(15)

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O5-H5W···O2[a]	0.99(5)	1.89(5)	2.846(3)	161(4)
O5-H5WA···N7[b]	1.07(7)	1.76(7)	2.824(3)	174(5)
O5-H5WA···N6[b]	1.07(7)	2.54(7)	3.499(3)	149(5)
O3-H3W···O1[c]	0.86(4)	1.91(4)	2.763(3)	170(3)
O4-H4WA···O2[c]	0.85(1)	1.88(1)	2.730(2)	177(3)
O3-H3WA···O1[d]	0.79(3)	1.96(3)	2.729(3)	161(3)
O4-H4W···O5	0.87(1)	1.80(1)	2.651(3)	167(3)

Symmetry codes:

For **1**: a -x+1,y+1/2,-z+1/2; b -x+1,-y+1,-z+1; c -x+1/2,y,-z+1; d -x+3/2,y,-z+1.

For **6**: a -x,-y+1,-z+1; b x,y,z+1; c -x+1,-y+1,-z+1; d x,y-1,z+1.

For **7**: a -x+2,-y,-z; b -x+1,-y,-z; c x,y+1,z-1; d x,y,z-1.

For **8**: a -x,-y+1,-z+1; b x,y+1,z-1; c -x,-y,-z+2; d -x,-y,-z+1; e x,y,z-1.

For **9**: a x,y,z+1; b -x+1,-y+1,-z+2; c -x+1,-y+1,-z+1; d x+1,y-1,z+1.