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SUPPORTING INFORMATION

Studies on Structure and Chirality of A-Motif in Adenosine Monophosphate Nucleotide Metal Coordination Complexes

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Table S1. Selected Bond Lengths for Complexes **1-3**.

Complex 1		Complex 2		Complex 3	
Bond	**Length/Å**	**Bond**	**Length/Å**	**Bond**	**Length/Å**
Cd1−O1[1]	2.405(3)	Mn1−O1	2.271(5)	Cd1−O1	2.368(3)
Cd1−O1	2.404(3)	Mn1−O1[2]	2.271(5)	Cd1−O2	2.292(3)
Cd1−O2	2.234(3)	Mn1−O2[2]	2.100(5)	Cd1−O3	2.348(3)
Cd1−O2[1]	2.234(3)	Mn1−O2	2.100(5)	Cd1−O4	2.240(3)
Cd1−N1	2.333(3)	Mn1−N1[2]	2.302(5)	Cd1−N1	2.347(4)
Cd1−N1[1]	2.333(3)	Mn1−N1	2.302(5)	Cd1−N2[3]	2.306(4)
P1−O2	1.499(3)	P1−O2	1.506(5)	P1−O4	1.519(3)
P1−O3	1.530(4)	P1−O3	1.525(6)	P1−O5	1.514(3)
P1−O4	1.504(4)	P1−O4	1.499(6)	P1−O6	1.513(3)
P1−O5	1.609(3)	P1−O5	1.609(5)	P1−O7	1.600(2)
O5−C13	1.431(6)	O5−C13	1.421(10)	O7−C13	1.427(4)
O6−C14	1.427(5)	O6−C14	1.424(9)	O8−C13	1.407(4)
O6−C17	1.424(6)	O6−C17	1.412(9)	O9−C15	1.406(4)
O7−C15	1.421(6)	O7−C15	1.426(9)	O10−C14	1.437(4)
N1−C1	1.353(6)	N1−C1	1.341(9)	O10−C16	1.426(4)
N1−C5	1.322(5)	N1−C5	1.316(9)	N1−C1	1.322(6)
N3−C17	1.447(5)	N3−C17	1.451(9)	N1−C5	1.325(6)
N3−C18	1.374(6)	N3−C18	1.362(9)	N2−C17	2.306(4)
N3−C20	1.389(6)	N3−C20	1.377(9)	N2−C10	1.351(6)
N4−C18	1.307(6)	N4−C18	1.303(10)	N2−C12	1.347(6)
N4−C19	1.388(6)	N4−C19	1.381(10)	N3−C16	1.465(4)
N5−C20	1.347(6)	N5−C20	1.354(9)	N3−C17	1.368(4)
N5−C21	1.313(7)	N5−C21	1.335(10)	N3−C19	1.382(4)
N6−C21	1.337(6)	N6−C21	1.331(10)	N4−C17	1.301(5)
N6−C22	1.358(7)	N6−C22	1.359(11)	N4−C18	1.380(5)
N7−C22	1.334(7)	N7−C22	1.344(10)	N5−C19	1.335(5)

Symmetry code: #1 2-x, 1-y, z; #2 1-x,1- y, +z; #3 +x, +y, 1+z.

Table S2. Selected Bond Angles for Complex **1**.

Angle	Angle/˚	Angle	Angle/˚
O1−Cd1−O1^{1}	91.23(15)	C5−C4−C3	119.6(4)
O2−Cd1−O1^{1}	174.72(17)	N1−C5−C4	123.2(4)
O2^{1}−Cd1−O1^{1}	87.69(12)	C6^{2}−C6−C3	125.5(5)
O2^{1}−Cd1−O1	174.72(17)	O5−C13−C14	109.7(4)
O2−Cd1−O1	87.69(12)	O6−C14−C13	109.8(4)
O2^{1}−Cd1−O2	93.85(17)	O6−C14−C15	106.5(4)
O2−Cd1−N1	96.64(13)	C13−C14−C15	117.2(4)
O2−Cd1−N1^{1}	90.93(13)	O7−C15−C14	108.6(4)
O2^{1}−Cd1−N1^{1}	96.64(13)	O7−C15−C16	112.2(4)
O2^{1}−Cd1−N1	90.93(13)	C14−C15−C16	101.6(4)
N1−Cd1−O1^{1}	88.37(14)	C17−C16−C15	102.6(4)
N1−Cd1−O1	83.88(14)	O6−C17−N3	106.9(4)
N1^{1}−Cd1−O1^{1}	83.88(14)	O6−C17−C16	105.8(4)
N1^{1}−Cd1−O1	88.37(14)	N3−C17−C16	115.6(4)
N1−Cd1−N1^{1}	168.92(16)	N4−C18−C3	114.2(4)
O2−P1−O3	111.2(2)	N4−C19−C22	131.9(5)
O2−P1−O4	114.8(2)	C20−C19−N4	111.4(4)
O2−P1−O5	108.9(2)	C20−C19−C22	116.7(5)
O3−P1−O5	104.2(2)	N5−C20−N3	127.0(4)
O4−P1−O3	112.2(3)	N5−C20−C19	127.3(5)
O4−P1−O5	104.6(2)	C19−C20−N3	105.7(4)
P1−O2−Cd1	135.5(2)	N5−C21−N6	129.6(5)
C13−O5−P1	117.2(3)	N6−C22−C19	117.3(5)
C17−O6−C14	110.3(4)	N7−C22−N6	119.8(5)
C1−N1−Cd1	119.5(3)	N7−C22−C19	122.9(6)
C5−N1−Cd1	122.2(3)	C7−N2−C11	120.0(5)
C5−N1−C1	118.1(3)	N2−C7−C8	121.2(6)
C18−N3−C17	127.7(4)	C7−C8−C9	121.7(6)
C18−N3−C20	105.1(4)	C8−C9−C10	117.1(5)
C20−N3−C17	126.8(4)	C8−C9−C12B	116.4(5)
C18−N4−C19	103.6(4)	C8−C9−C12A	146.4(11)
C21−N5−C20	110.6(4)	C10−C9−C12B	126.5(6)
C21−N6−C22	118.5(4)	C10−C9−C12A	96.2(11)
N1−C1−C2	122.4(4)	C11−C10−C9	119.6(6)
C1−C2−C3	119.6(4)	N2−C11−C10	120.5(5)

Symmetry code: #1 2-x, 1-y, +z.

Table S3. Selected Hydrogen Bonds for Complex **1** and Complex **2**.

Complex 1

D–H–A	d(D–H)/Å	d(H···A)/Å	d(D–A)/Å	D–H–A/°
O1–H1A···O4	0.89	1.95	2.767(5)	151
O3–H3···N2	0.82	1.79	2.536(6)	151
O7–H7···O10[1]	0.82	1.99	2.789(8)	165
N7–H7B···N4[2]	0.86	2.21	3.015(7)	156

Symmetry code: #1 1+x, +y, +z; #2 2-x, 2-y, z.

Complex 2

D–H–A	d(D–H)/Å	d(H···A)/Å	d(D–A)/Å	D–H–A/°
O1–H1B···O4	0.85	1.99	2.783(8)	155
O3–H3···N2	0.82	1.71	2.516(9)	167
O7–H7···O10[1]	0.82	2.06	2.863(15)	168
N7–H7B···N4[2]	0.86	2.18	2.995(9)	156

Symmetry code: #1 -x, y, 1+z; #2 1-x, -y, z.

Table S4. Selected Bond Angles for Complex **2**.

Atoms	Angle/˚	Atoms	Angle/˚
$O1^1$–Mn1–O1	88.6(3)	C3–C4–C5	119.0(7)
O1–Mn1–$N1^1$	88.8(2)	N1–C5–C4	124.0(7)
O1–Mn1–N1	83.5(2)	$C6^2$–C6–C3	125.9(9)
$O1^1$–Mn1–$N1^1$	83.5(2)	O5–C13–C14	110.3(7)
$O1^1$–Mn1–N1	88.8(2)	O6–C14–C13	110.9(7)
O2–Mn1–$O1^1$	173.0(2)	O6–C14–C15	106.2(6)
$O2^1$–Mn1–$O1^1$	87.95(18)	C15–C14–C13	115.5(7)
O2–Mn1–O1	87.95(18)	O7–C15–C14	108.4(7)
$O2^1$–Mn1–O1	173.0(2)	O7–C15–C16	112.3(6)
O2–Mn1–$O2^1$	96.2(3)	C14–C15–C16	102.8(6)
O2–Mn1–N1	96.9(2)	C17–C16–C15	101.5(6)
O2–Mn1–$N1^1$	90.3(2)	O6–C17–N3	107.4(6)
$O2^1$–Mn1–N1	90.3(2)	O6–C17–C16	105.7(6)
$O2^1$–Mn1–N1	96.9(2)	N3–C17–C16	115.4(6)
$N1^1$–Mn1–N1	169.2(3)	N4–C18–C3	114.3(7)
O2–P1–O3	110.9(3)	N4–C19–C22	132.5(8)
O2–P1–O5	109.7(3)	C20–C19–N4	111.3(6)
O5–P1–O5	104.1(3)	C20–C19–C22	116.2(8)
O4–P1–O2	114.1(3)	N5–C20–N3	126.8(6)
O4–P1–O3	113.4(4)	N5–C20–C19	127.7(7)
O4–P1–O5	104.0(3)	C19–C20–N3	105.5(6)
P1–O2–Mn1	139.0(3)	N5–C21–N6	129.4(8)
C13–O5–P1	117.9(5)	N6–C22–C19	118.7(8)
C17–O6–C14	110.6(6)	N7–C22–N6	118.8(7)
C1–N1–Mn1	120.4(5)	N7–C22–C19	122.5(8)
C5–N1–Mn1	122.6(5)	C7–N2–C11	119.3(8)
C5–N1–C1	116.9(6)	N2–C7–C8	122.0(9)
C18–N3–C17	127.0(6)	C7–C8–C9	120.9(10)
C18–N3–C20	105.5(6)	C8–C9–C10	117.3(9)
C20–N3–C17	127.1(6)	C8–C9–C12B	145(2)
C18–N4–C19	103.4(6)	C8–C9–C12A	110.7(16)
C21–N5–C20	110.0(6)	C10–C9–C12B	97(2)
C21–N6–C22	117.9(6)	C10–C9–C12A	132.0(17)
N1–C1–C2	123.9(7)	C11–C10–C9	119.0(9)
C1–C2–C3	118.8(7)	N2–C11–C10	121.5(9)

Symmetry code: #1 2-x, 1-y, +z.

Table S5. Selected Bond Angles for Complex **3**.

Atoms	Angle/˚	Atoms	Angle/˚
O2−Cd1−O1	83.39(12)	C2−C3−C6	122.8(4)
O2−Cd1−O3	169.44(11)	C4−C3−C2	117.3(4)
O2−Cd1−N1	90.18(14)	C4−C3−C6	119.9(4)
O2−Cd1−N2^{1}	86.07(13)	C3−C4−C5	120.6(4)
O3−Cd1−O1	87.59(11)	N1−C5−C4	121.7(4)
O4−Cd1−O1	170.34(10)	C7−C6−C3	126.1(4)
O4−Cd1−O2	102.07(11)	C6−C7−C8	124.5(4)
O4−Cd1−O3	87.64(11)	C9−C8−C7	119.6(4)
O4−Cd1−N1	86.54(13)	C11−C8−C7	123.7(4)
O4−Cd1−N2^{1}	98.13(12)	C11−C8−C9	116.7(4)
N1−Cd1−O1	85.47(12)	C10−C9−C8	120.0(4)
N1−Cd1−O3	94.57(14)	N2−C10−C9	123.0(4)
N2^{1}−Cd1−O1	90.14(12)	C8−C11−C12	120.5(4)
N2^{1}−Cd1−O3	88.48(13)	N2−C12−C11	122.6(4)
N2^{1}−Cd1−N1	174.53(16)	O7−C13−C14	109.1(2)
O4−P1−O7	102.47(16)	O10−C14−C13	109.3(3)
O5−P1−O4	111.99(16)	O10−C14−C23	104.0(2)
O5−P1−O7	108.12(17)	C13−C14−C23	116.1(3)
O6−P1−O4	112.73(19)	O9−C15−C16	110.9(3)
O6−P1−O5	113.4(2)	O9−C15−C23	107.7(3)
O6−P1−O7	107.29(19)	C23−C15−C16	102.2(3)
P1−O4−Cd1	135.00(18)	O10−C16−N3	108.1(3)
C1−N1−Cd1	119.6(2)	O10−C16−C15	107.0(3)
C13−O7−P1	109.6(2)	N3−C16−C15	113.7(3)
C16−O10−C14	123.1(3)	N4−C17−N3	113.8(3)
C1−N1−Cd1	117.9(4)	N4−C18−C19	110.7(3)
C1−N1−C5	119.0(3)	N4−C18−C21	133.3(3)
C10−N2−Cd1^{2}	123.5(3)	C19−C18−21	116.0(4)
C12−N2−Cd1^{2}	119.5(3)	N3−C19−C18	105.3(3)
C12−N2−C10	117.0(4)	N5−C19−N3	127.7(3)
C17−N3−C16	128.6(3)	N5−C19−C18	126.9(3)
C17−N3−C19	105.8(3)	N6−C20−N5	128.2(4)

Atoms	Angle/˚	Atoms	Angle/˚
C19−N3−C16	125.6(3)	N6−C21−C18	118.4(4)
C17−N4−C18	104.4(3)	N7−C21−N6	119.0(4)
C19−N5−C20	111.5(3)	N7−C21−C18	122.6(5)
C20−N6−C21	118.9(4)	O8−C23−C18	112.1(2)
N1−C1−C2	123.8(5)	O8−C23−C15	114.8(3)
C1−C2−C3	118.5(4)	C15−C23−C14	101.6(3)

Symmetry code: #1 +x, +y, 1+z.

Table S6. Selected Hydrogen Bonds for Complex **3**.

D−H···A	d(D−H)/Å	d(H···A)/Å	d(D−A)/Å	D−H−A/°
O2−H2A···O13	0.94	2.07	2.746(4)	159
O2−H2B···O14	0.94	1.91	2.755(5)	154
O8−H8···O5[1]	0.82	1.85	2.719(4)	161
O9−H9···O15[2]	0.86	1.87	2.730(7)	167
N7−H7B···O17	0.85	2.12	2.892(7)	148
O11−H11A···O6	0.85	1.94	2.725(5)	162
O11−H11B···N6[3]	0.85	1.85	2.804(5)	148
O13−H13C···O12	0.85	1.91	2.725(5)	146
O13−H13D···O11[4]	0.85	1.94	2.733(5)	153

Symmetry code: #1 -1+x, +y, +z; #2 -1+x, -1+y, z; #3 +x, -1+y, -1+z; #4 +x, y+1, +z.

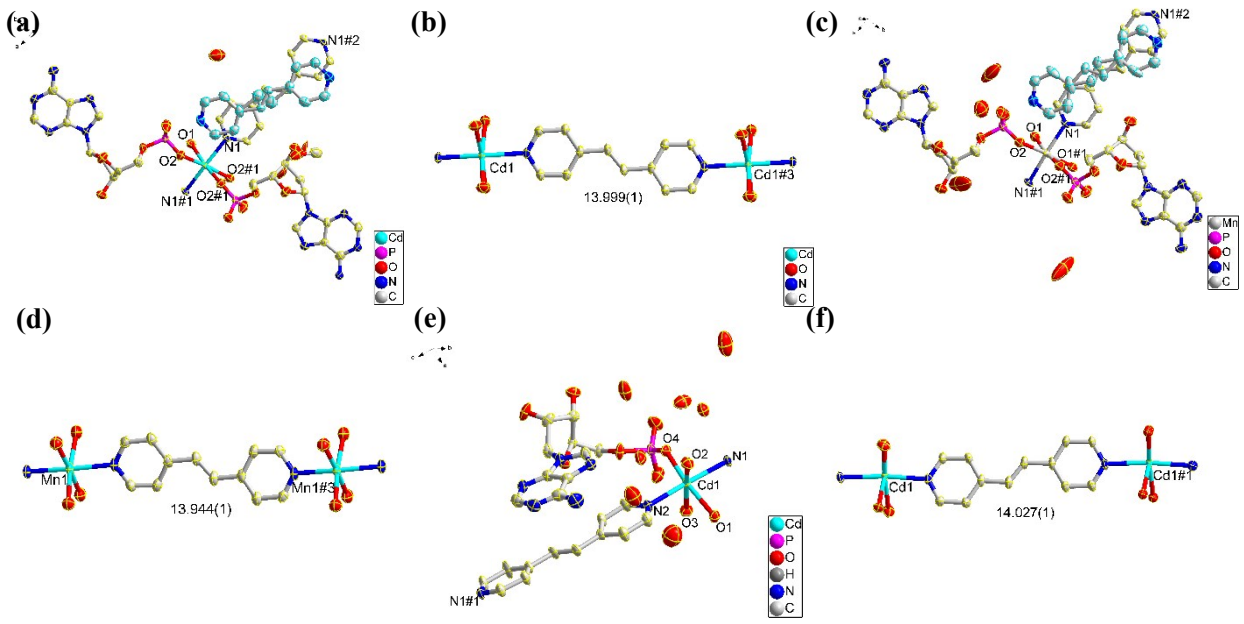

Fig. S1. The coordination environment of metal in molecular structure with solvent molecules (a) in Complex **1**, (b) distance between Cd-Cd in complex **1** is 13.999(1) Å (Symmetry code: #1 2-x, 1-y, z; #2 1-x, 1-y, z; #3 -1+x, y, z); (c) in Complex **2**, (d) distance between Mn1-Mn1 in complex **2** is 13.944(1) Å (Symmetry code: #1 2-x, 1-y, z; #2 1-x, 1-y, z; #3 -1+x, y, z); (e) in Complex **3**, (f) distance between Cd-Cd in complex **2** is 14.027(1) Å(Symmetry code: #1 x, y, 1+z).

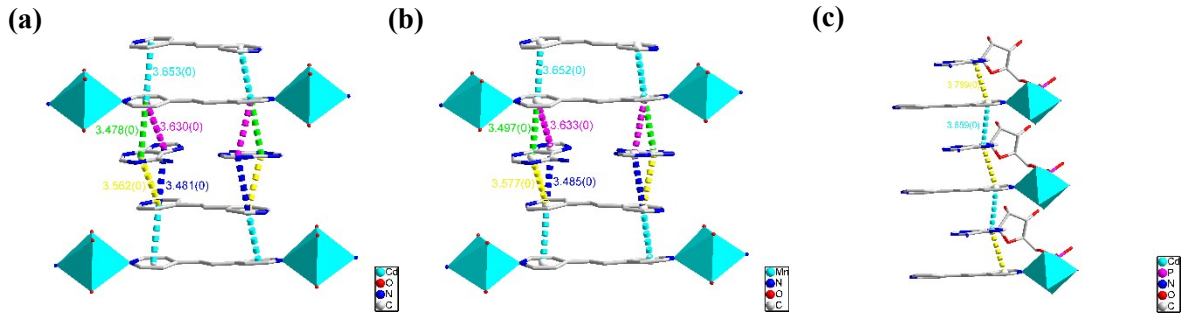

Fig. S2. The molecular structure with parallel distances between **(a)** Bpe-Adenine bases is 3.478(0) Å, 3.630(0) Å, 3.562(0) Å, 3.478(0) Å and Bpe-Bpe is 3.653(0) Å in Complex **1** (**b)** Bpe-Adenine bases are 3.497(0) Å, 3.633(0) Å, 3.577(0) Å, 3.485(0) Å and Bpe-Bpe is 3.652(0) Å in Complex **2 (c)** Bpe-Adenine base is 3.789(0) Å and 3.659(0) Å in Complex **3**.

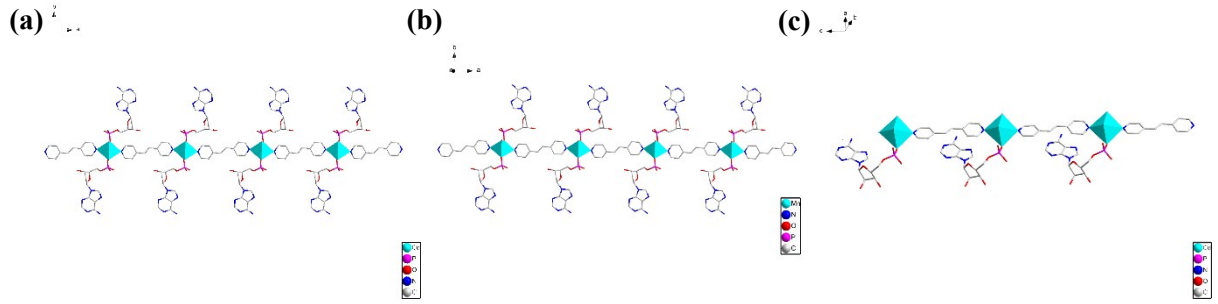

Fig. S3: 1D chain based on bridging ligand (Bpe) with side arms of Nucleotide ligand in **(a)** Complex **1** (dAMP-Cd-Bpe) **(b)** Complex **2** (dAMP-Mn-Bpe) and **(c)** Complex **3** (AMP-Cd-Bpe).

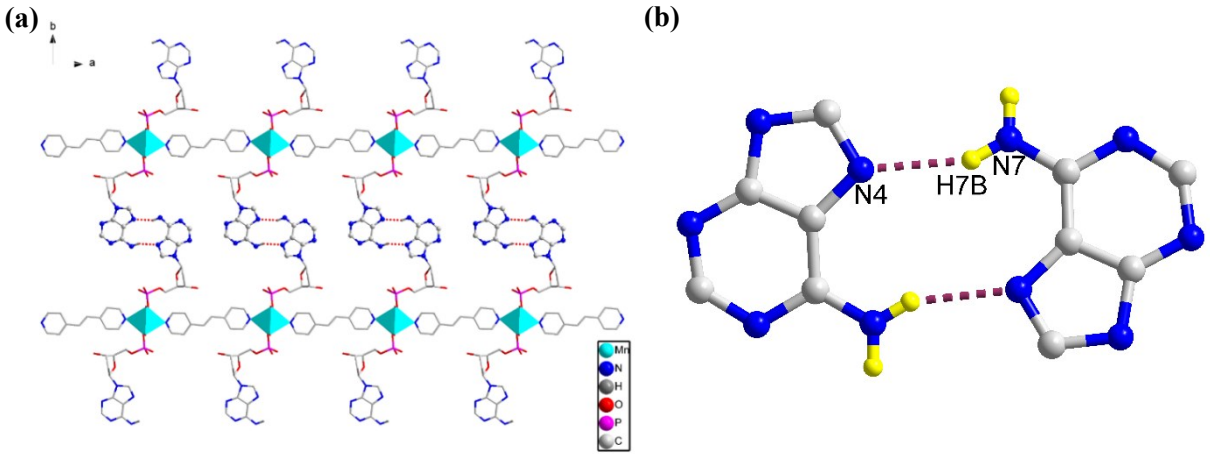

Fig. S4: Complex **1**(dAMP-Cd-BPE) and Complex **2** (AMP-Cd-Bpe) are isostructural **(a)** purine bases showing formation of A-Motif by hydrogen bonding in complex **2 (b)** Structure of A-Motif showing the Distances between Hydrogen bonded atoms of purine bases in complex **2**.

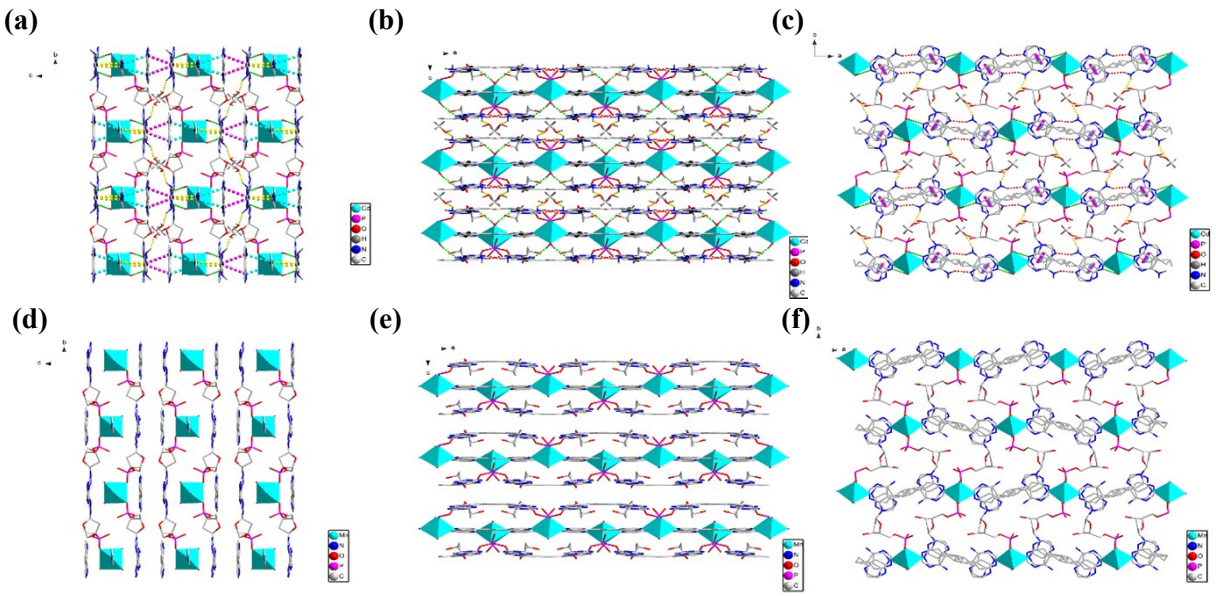

Fig. S5: 3D Supramolecular framework of complexes with Hydrogen bonding and pi-pi interactions (Bpe-Bpe, Bpe-Adenine, Adenine-Adenine bases) among different layers in *a, b, c*-view of **(a-c)** Complex **1** (dAMP-Cd-Bpe) **(d-f)** Complex **2** (dAMP-Mn-Bpe).

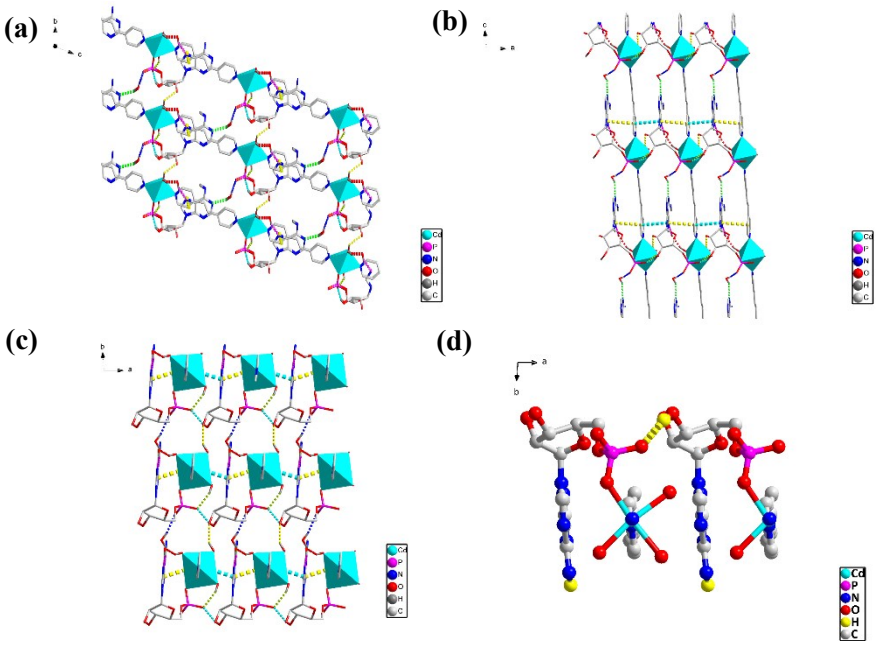

Fig. S6: 3D Supramolecular framework of complexes with Hydrogen bonding and pi-pi interactions (Bpe-Bpe, Bpe-Adenine, Adenine-Adenine bases) among different layers in *a, b, c*-view of **(a-c)** Complex **3** (AMP-Cd-Bpe) **(d))** Hydrogen bonding between two layers in Complex **3** (AMP-Cd-Bpe).

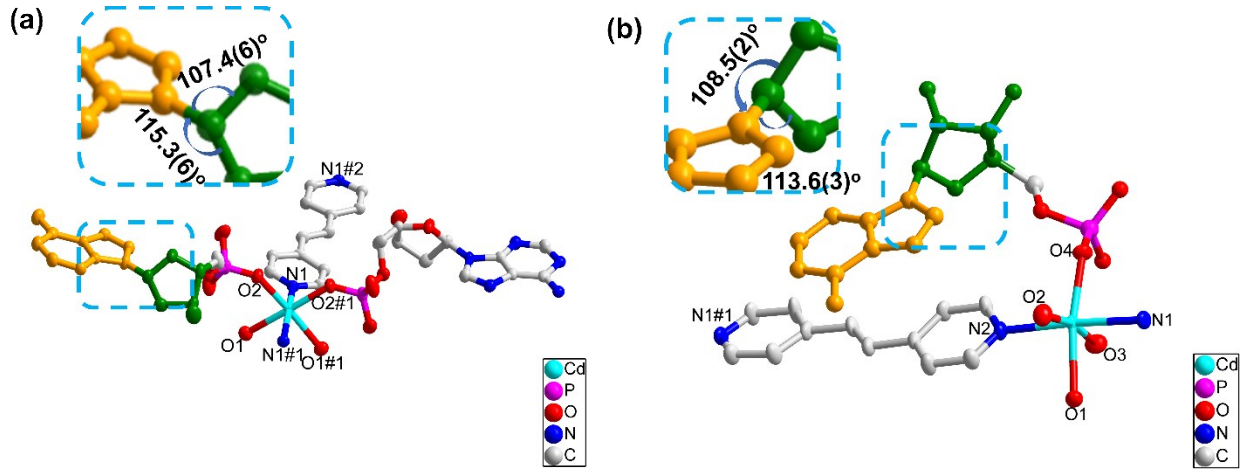

Fig. S7: Angle between pentose ring and adenine base of complex **2 (a)**, complex **3 (b)**. Symmetry code in (a): #1 2-x, 1-y, +z; #2 1-x, 1-y, +z. Symmetry code in (b): #1 x, y, 1+z

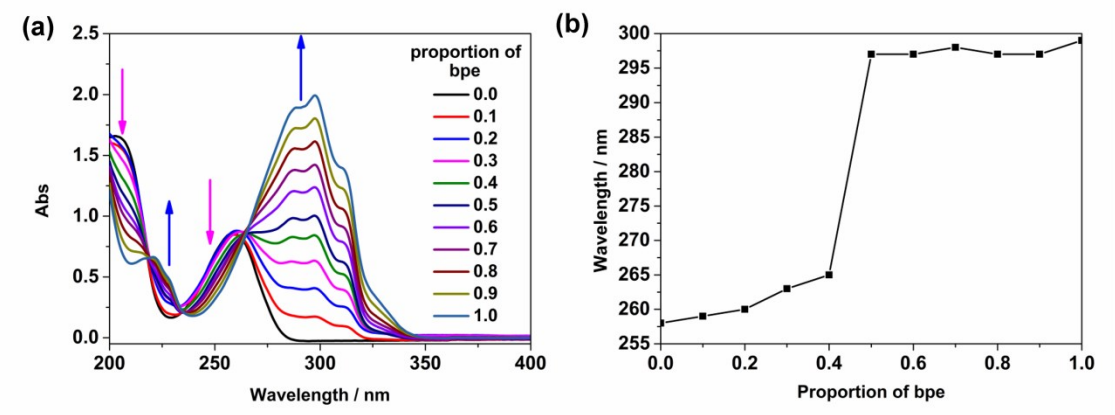

Fig. S8: (a) UV/Vis spectroscopy titration of Mn–AMP (1:1) upon addition of bpe. The total concentration of AMP and bpe is held fixed (3.75×10^{-5} M) varying the ratio of the components bpe. (b) Plot of the compound formation of Mn–AMP with bpe monitored with UV/vis spectra.

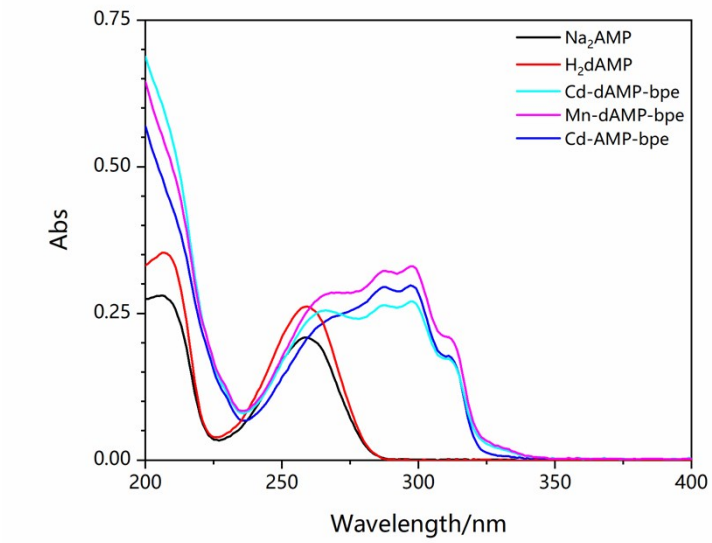

Fig. S9: UV/vis absorption spectra of AMP, dAMP and their coordination complexes with Mn(II) and Co(II) ions. The spectra were obtained by measuring approximately 1.0×10^{-5} mol·L^{-1} solution in 1 cm cell.

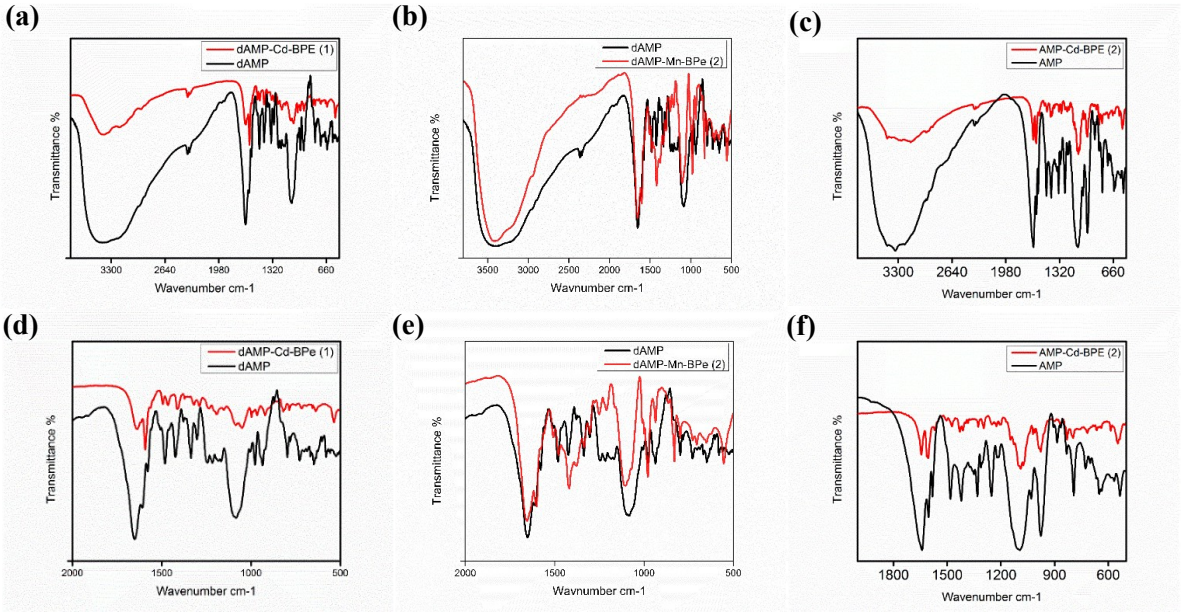

Fig. S10: Comparison of Infrared spectrum measured from wavenumber in range of 4000-500 cm^{-1} and 2000-500 cm^{-1} **(a)** IR spectra of dAMP (Black), dAMP-Cd-Bpe (Complex **1**) (red). **(b)** IR spectra of dAMP (Black), dAMP-Mn-Bpe (Complex **1**) (red). **(c)** IR spectra of AMP (Black) and AMP-Cd-Bpe (Complex **2**) (Red) showing match with each other prove the presence of AMP in Complexes **(d)** Showing the IR (2000-500cm^{-1}) of dAMP and Complex**1**, **(e)** dAMP-Complex **2** and **(f)** AMP-Complex **3**.

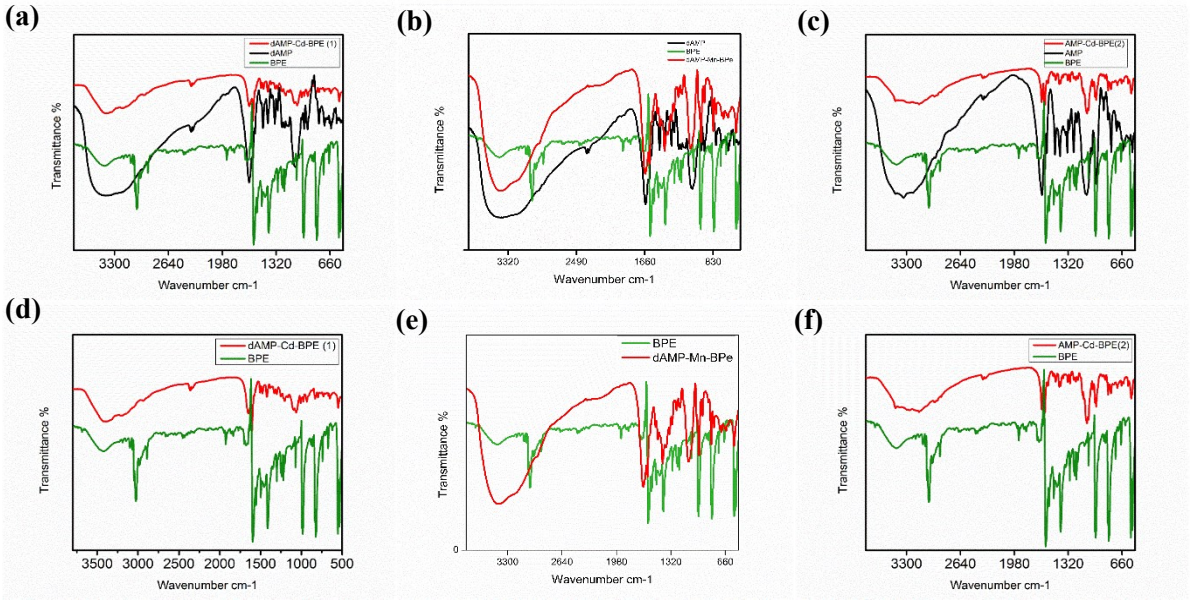

Fig. S11: (a) IR spectra of dAMP (Black), Bpe (Green) and dAMP-Cd-Bpe (Complex **1**) (Red) **(b)** IR spectra of dAMP (Black), Bpe (Green) and dAMP-Mn-Bpe (Complex **2**) (Red) **(c)** IR spectra of AMP (Black), Bpe (Green) and AMP-Cd-Bpe (Complex **3**) (Red) **(d)** IR spectra of Bpe (Green) dAMP-Cd-Bpe (Complex **1**) (red) **(e)** IR spectra of Bpe (Green) dAMP-Mn-Bpe (Complex **1**) (red) **(f)** IR spectra of Bpe (Green) AMP-Cd-Bpe (Complex **3**) (red). A new absorption peak around 1500 cm^{-1} and 1100cm^{-1}appeared in spectra of complex **1**-**3**.

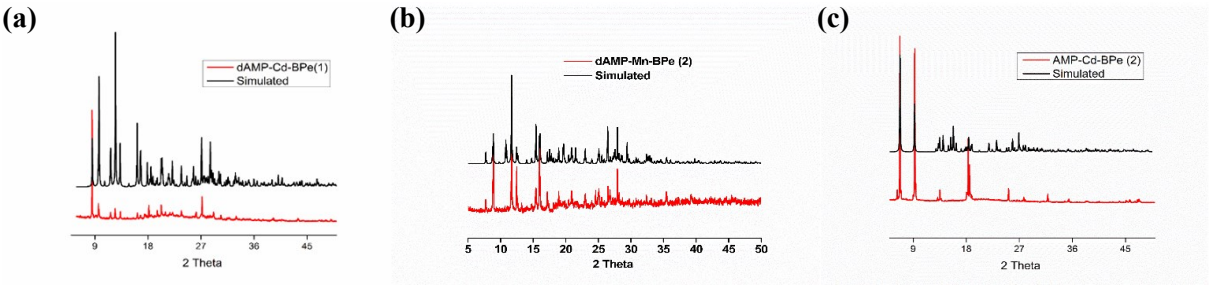

Fig. S12: X-ray powder diffraction (PXRD) measurements as a pure phase, similar with their single crystals. PXRD patterns show the comparison between the experimental value and Simulated for complex**1 (a)** Complex **2 (b)** and Complex **3 (c)**.

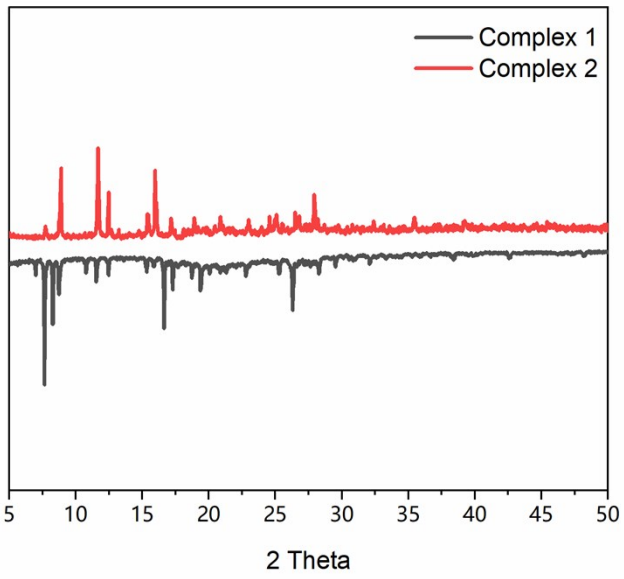

Fig. S13: X-ray powder diffraction (PXRD) for complex**1** and Complex **2**.